# Making Programming Synonymous with Parallel Programming for Linear Algebra

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#### The Current Core FLAME Team

- UT-Austin
  - Ernie Chan
  - Victor Eijkhout
  - Kazushige Goto
  - Field Van Zee
  - (this list is a bit out of date)
- UJI-Spain
  - Enrique Quintana-Orti
  - Gregorio Quintana-Orti
- Aachen University
  - Paolo Bientinesi
- Others
  - See <a href="http://www.cs.utexas.edu/users/flame">http://www.cs.utexas.edu/users/flame</a>

# The presented work is also in collaboration with

- Maribel Castillo
- Francisco D. Igual
- Rafael Mayo

(Univ. Jaume I, Spain)

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- Unrestricted grants from NEC, Dr. Truchard (CEO of National Instruments)
- For a little \$\$\$ UTK's or DOE's name could be here...

#### What is FLAME

- A notation for representing algorithms
- A methodology for deriving correct algorithms
- APIs for representing algorithms in code
- A library (libFLAME)
- A pedagogical tool

#### In other words:

FLAME is a programmer's lifestyle choice

### The Need for Forward Compatibility

- An operation is encountered for which no library routine exists
- A novel architecture comes along
- The traditional library does not deliver the performance one wants
- A novel data storage scheme comes along

What we need is a flexible infrastructure

#### Motivating scenario

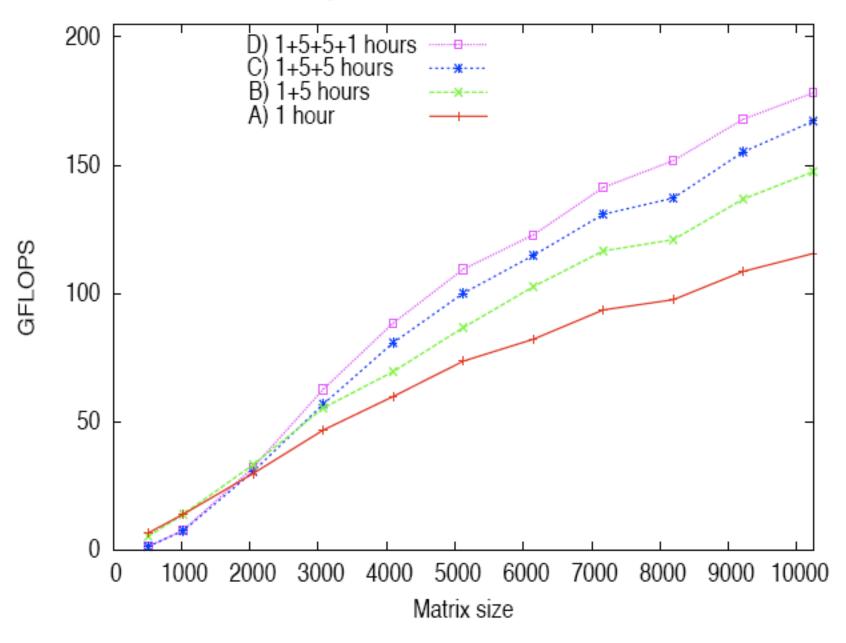
- A new architecture comes along. How much effort does it take to port a typical library routine to this architecture?
  - NVIDIA Tesla S870 system
    - 4 NVIDIA G80 GPUs
    - 6 Gbytes DDR3 memory
    - Peak 1.4 Tflops single precision
    - Available libraries: sequential CUBLAS 1.1 (later 2.0)
    - Host: Intel Xeon QuadCore E5405 (2.0 GHz)
      - Two PCIExpress Gen2 interfaces
         (peak bandwidth: 48 Gbytes/sec per interface)

#### What do we have to do?

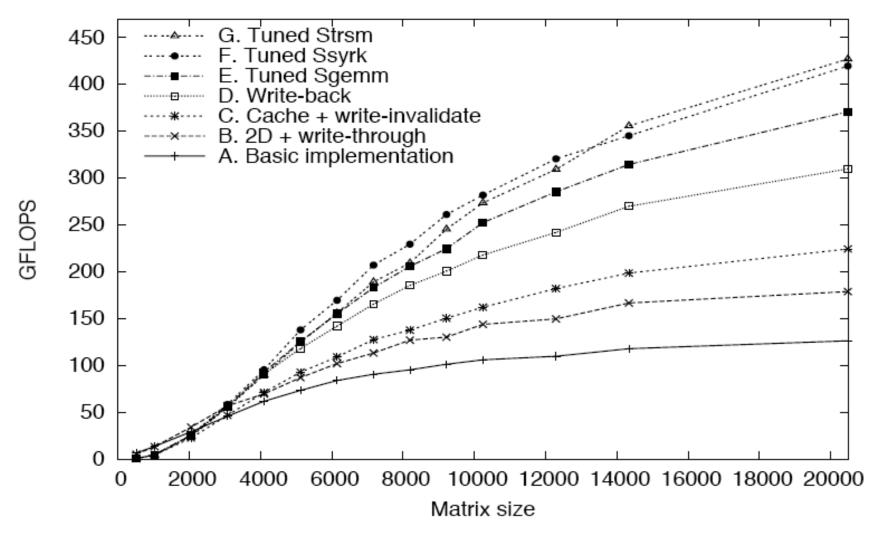
- View the matrix as a collection of blocks that are stored contiguously
  - This is (thought to be) hard
- Program the algorithm as an algorithm-by-blocks
  - This is (thought to be) hard
- Schedule the operations with blocks and manage the movement of blocks between the host and the GPUs
  - This is (thought to be) hard

#### Welcome to programming hell

#### Cholesky factorization on NVIDIA Tesla S870



#### Cholesky factorization on NVIDIA Tesla S870



#### Overview

- A bit of history
- Programming algorithms-by-blocks is hard easy
  - An example: Cholesky factorization by blocks
- Programming algorithms-by-blocks further simplifies complicates programming (future) multicore architectures
- Conclusion
- Resources

#### Overview

- A bit of history
- Programming algorithms-by-blocks is hard easy
  - An example: Cholesky factorization by blocks
- Programming algorithms-by-blocks further simplifies complicates programming (future) multicore architectures
- Conclusion
- Resources

#### A Bit of History

### Once upon a time there was package...

- 1972: EISPACK
  - Package for the solution of the dense eigenvalue problem
    - E.g.: A  $x = \lambda x$
  - First robust software pack
    - Numerical stability, performance, and portability were a concern
    - Consistent formatting of code
  - Coded in Algol
  - First released in 1972

#### Basic Linear Algebra Subprograms (BLAS)

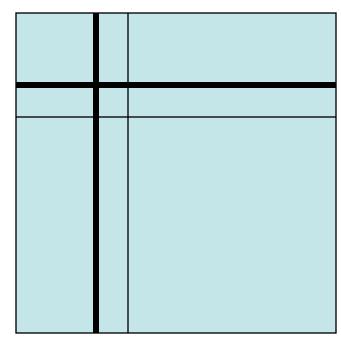
- In the 1970s vector supercomputers ruled
- Dense (and many sparse) linear algebra algorithms can be formulated in terms of vector operations
- By standardizing an interface to such operations, portable high performance could be achieved
  - Vendors responsible for optimized implementations
  - Other libraries coded in terms of the BLAS
- First proposed in 1973. Published in C. L. Lawson, R. J. Hanson, D. Kincaid, and F. T. Krogh, Basic Linear Algebra Subprograms for FORTRAN usage, ACM Trans. Math. Soft., 5 (1979).
- Later became known as the level-1 BLAS
- Fortran77 interface

# Linear Algebra Package (LINPACK)

- Targeted solution of linear equations and linear least-squares
- Coded in terms of the level-1 BLAS for portability
- Started in 1974. Published/released in 1977

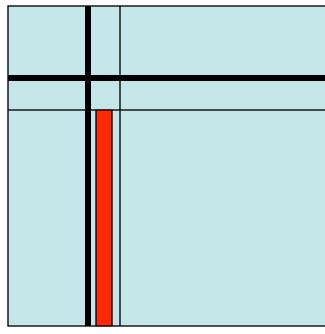
J. J. Dongarra, J. R. Bunch, C. B. Moler and G. W. Stewart. LINPACK User's Guide, SIAM, 1977

Fortran66 interface



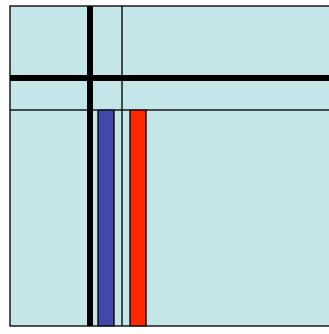
June 19, 2008

```
do 60 k = 1, nm1
      kp1 = k + 1
      1 = idamax(n-k+1, a(k, k), 1) + k - 1
      ipvt(k) = 1
      if (a(1,k) .eq. 0.0d0) go to 40
         if (l .eq. k) qo to 10
            t = a(1,k)
            a(1,k) = a(k,k)
            a(k,k) = t
10
         continue
         t = -1.0d0/a(k,k)
         call dscal(n-k,t,a(k+1,k),1)
         row elimination with column indexing
         do 30 j = kp1, n
            t = a(1,j)
            if (1 .eq. k) go to 20
               a(1,j) = a(k,j)
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            continue
            call daxpy (n-k, t, a(k+1, k), 1, a(k+1, j), 1)
30
         continue
      go to 50
40
      continue
         info = k
      continue
60 continue
```



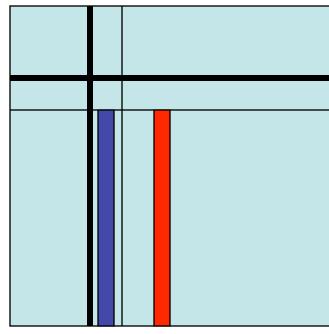
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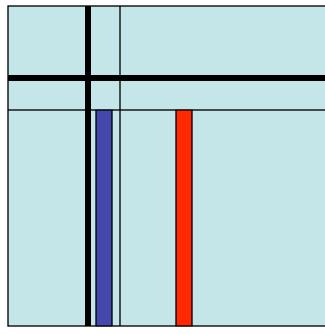
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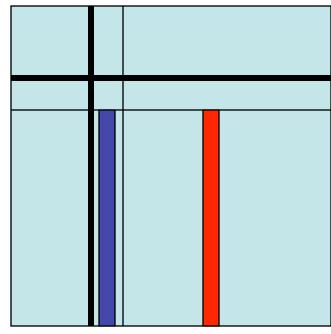
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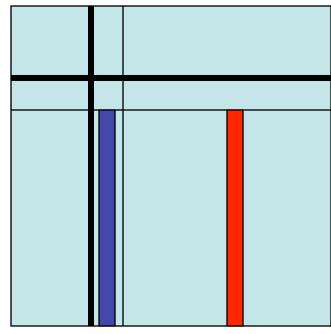
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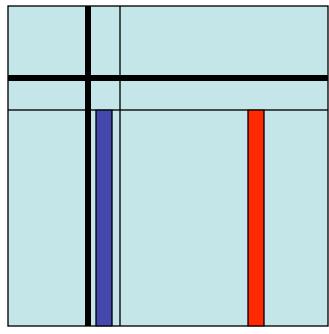
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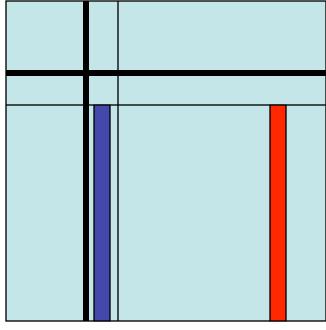
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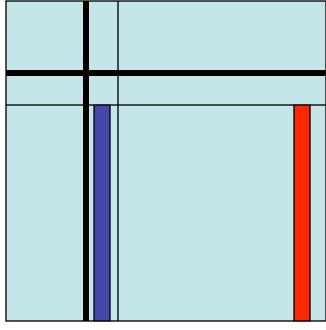
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June 19, 2008
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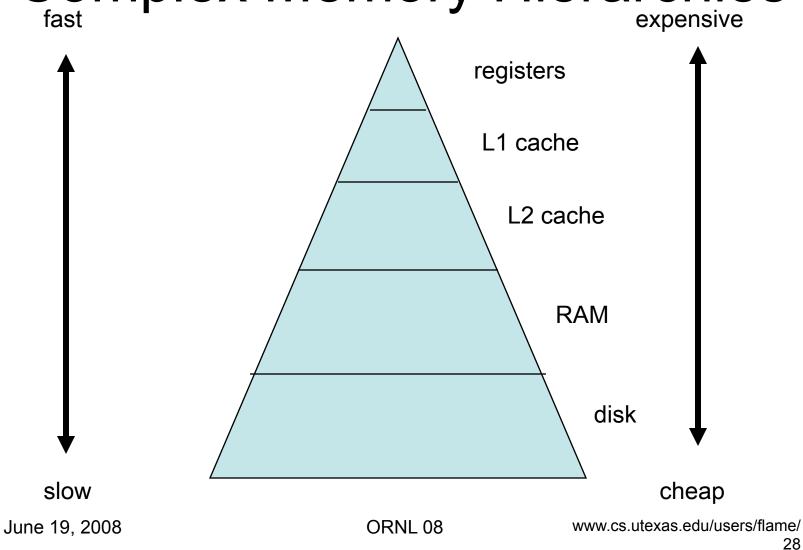
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         continue
      go to 50
40
      continue
         info = k
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```

#### LINPACK (continued)

- Portable high performance on vector architectures
- Poor performance when architectures with complex memory hierarchies arrived in the 1980s
  - O(n) operations on O(n) data means bandwidth to main memory becomes the limiting factor

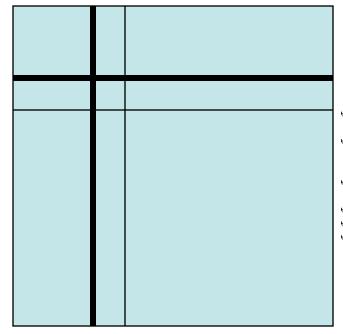
#### Complex Memory Hierarchies expensive



### Evolving Towards Higher Performance

- Level 2 BLAS: matrix-vector operations
  - Started in 1984. Published in 1988
    - J. J. Dongarra, J. Du Croz, S. Hammarling, and R. J. Hanson, *An extended set of FORTRAN Basic Linear Algebra Subprograms*, <u>ACM Trans. Math. Soft., 14 (1988)</u>, pp. 1--17.
  - Casts computation in terms of operations like matrix-vector multiplication and rank-1 update
  - Benefit: vector(s) can be kept in cache memory
  - Problem: O( n² ) operations on O(n² ) data

LAPACK
LU factorization
with partial pivoting
unblocked algorithm
(abbreviated)

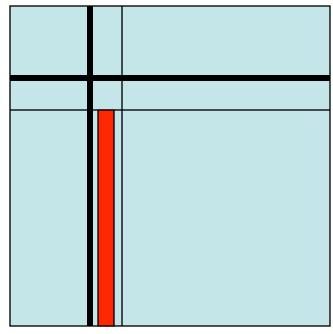


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```
DO 10 J = 1, MIN( M, N )
      JP = J - 1 + IDAMAX(M-J+1, A(J, J), 1)
      IPIV(J) = JP
      IF ( A ( JP, J ).NE.ZERO ) THEN
         IF ( JP.NE.J )
  $
            CALL DSWAP( N, A( J, 1 ), LDA, A( JP, 1 ), LDA )
         IF ( J.LT.M ) THEN
            IF ( ABS (A ( J, J )) .GE. SFMIN ) THEN
               CALL DSCAL( M-J, ONE / A( J, J ), A( J+1, J ), 1 )
            ELSE
              DO 20 I = 1, M-J
                 A(J+I, J) = A(J+I, J) / A(J, J)
20
              CONTINUE
            END IF
         END IF
      ELSE IF ( INFO.EQ. 0 ) THEN
         INFO = J
      END IF
      IF ( J.LT.MIN ( M, N ) ) THEN
         Update trailing submatrix.
         CALL DGER( M-J, N-J, -ONE, A( J+1, J ), 1, A( J, J+1 ), LDA,
                    A(J+1, J+1), LDA)
      END IF
10 CONTINUE
```

ORNL 08

# LAPACK LU factorization with partial pivoting unblocked algorithm (abbreviated)

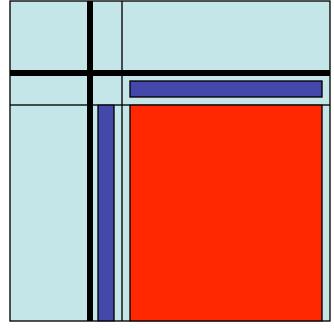


June 19, 2008

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              DO 20 I = 1, M-J
                A(J+I, J) = A(J+I, J) / A(J, J)
20
              CONTINUE
            END IF
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      IF ( J.LT.MIN ( M, N ) ) THEN
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         CALL DGER( M-J, N-J, -ONE, A( J+1, J ), 1, A( J, J+1 ), LDA,
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10 CONTINUE
```

ORNL 08

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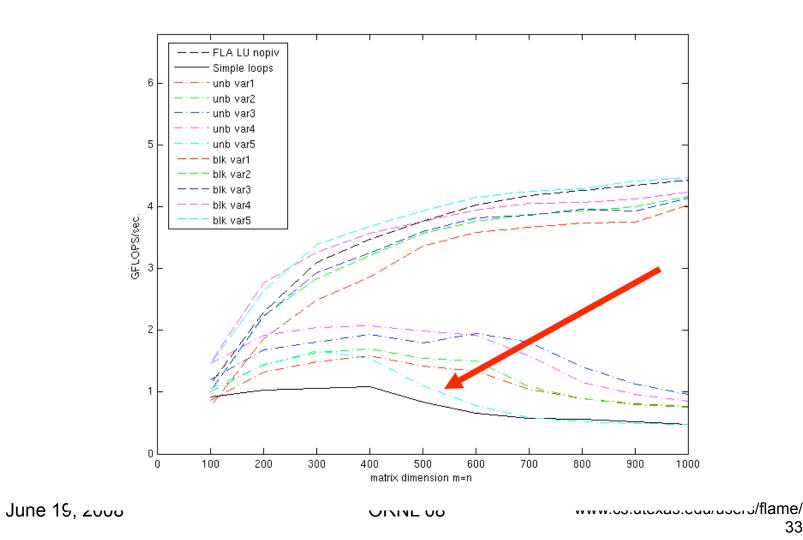


June 19, 2008

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DO 10 J = 1, MIN( M, N )
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ORNL 08

#### Performance (Intel Xeon 3.4GHz)



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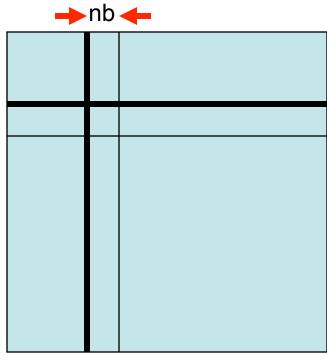
### Evolving Towards High Performance

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  - Started in 1986. Published in 1990

J. J. Dongarra, J. Du Croz, I. S. Duff, and S. Hammarling, A set of Level 3 Basic Linear Algebra Subprograms, ACM Trans. Math. Soft., 16 (1990)

- Casts computation in terms of operations like matrix-matrix multiplication
- Benefit: submatrices can be kept in cache
- O( n<sup>3</sup> ) operations on O(n<sup>2</sup> ) data

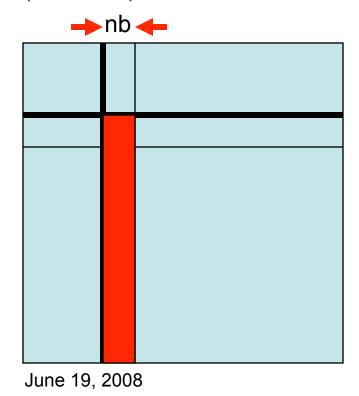
# LAPACK LU factorization with partial pivoting blocked algorithm (abbreviated)



June 19, 2008

```
DO 20 J = 1, MIN(M, N), NB
         JB = MIN(MIN(M, N) - J + 1, NB)
         CALL DGETF2( M-J+1, JB, A( J, J ), LDA, IPIV( J ), IINFO )
         IF( INFO.EQ.O .AND. IINFO.GT.O )
  $
            INFO = IINFO + J - 1
         DO 10 I = J, MIN(M, J+JB-1)
            IPIV(I) = J - 1 + IPIV(I)
10
         CONTINUE
         CALL DLASWP( J-1, A, LDA, J, J+JB-1, IPIV, 1 )
         IF ( J+JB.LE.N ) THEN
            CALL DLASWP( N-J-JB+1, A( 1, J+JB ), LDA, J, J+JB-1,
  $
                         IPIV, 1)
            CALL DTRSM( 'Left', 'Lower', 'No transpose', 'Unit', JB,
  $
                        N-J-JB+1, ONE, A(J, J), LDA, A(J, J+JB),
                        LDA )
            IF ( J+JB.LE.M ) THEN
               CALL DGEMM ( 'No transpose', 'No transpose', M-J-JB+1,
 $
                           N-J-JB+1, JB, -ONE, A( J+JB, J ), LDA,
  $
                           A( J, J+JB ), LDA, ONE, A( J+JB, J+JB ),
                           LDA )
            END IF
         END IF
20
      CONTINUE
```

# LAPACK LU factorization with partial pivoting blocked algorithm (abbreviated)

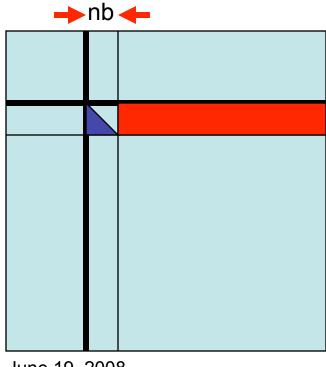


```
CALL DGETF2( M-J+1, JB, A( J, J ), LDA, IPIV( J ), IINFO )
        IF ( INFO.EQ.U .AND. IINFO.GT.U )
  $
            INFO = IINFO + J - 1
         DO 10 I = J, MIN(M, J+JB-1)
            IPIV(I) = J - 1 + IPIV(I)
10
         CONTINUE
         CALL DLASWP( J-1, A, LDA, J, J+JB-1, IPIV, 1 )
         IF ( J+JB.LE.N ) THEN
            CALL DLASWP( N-J-JB+1, A( 1, J+JB ), LDA, J, J+JB-1,
  $
                         IPIV, 1)
            CALL DTRSM( 'Left', 'Lower', 'No transpose', 'Unit', JB,
  $
                        N-J-JB+1, ONE, A(J, J), LDA, A(J, J+JB),
                        LDA )
            IF ( J+JB.LE.M ) THEN
               CALL DGEMM ( 'No transpose', 'No transpose', M-J-JB+1,
  $
                           N-J-JB+1, JB, -ONE, A( J+JB, J ), LDA,
  $
                           A( J, J+JB ), LDA, ONE, A( J+JB, J+JB ),
                           LDA )
            END IF
         END IF
20
      CONTINUE
```

DO 20 J = 1, MIN(M, N), NB

JB = MIN(MIN(M, N) - J + 1, NB)

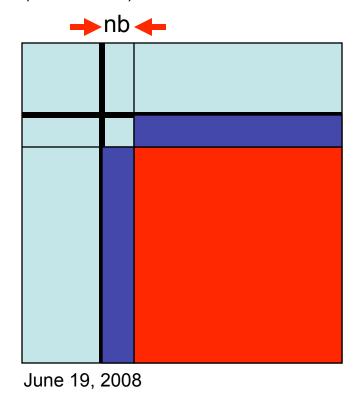
#### LAPACK LU factorization with partial pivoting blocked algorithm (abbreviated)



```
June 19, 2008
```

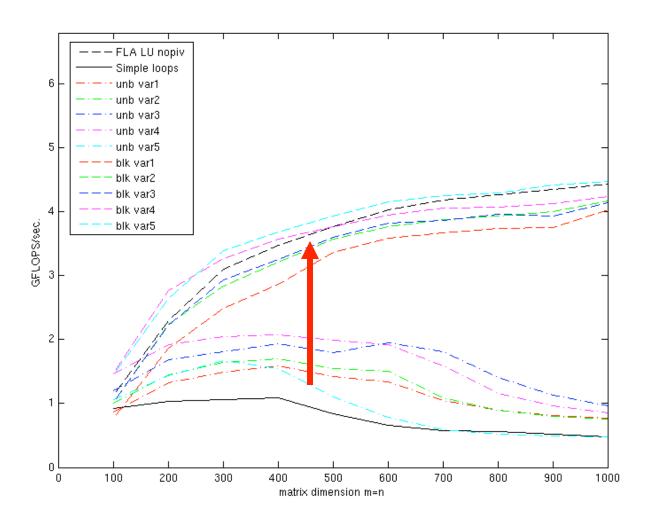
```
DO 20 J = 1, MIN(M, N), NB
         JB = MIN(MIN(M, N) - J + 1, NB)
         CALL DGETF2( M-J+1, JB, A( J, J ), LDA, IPIV( J ), IINFO )
        IF( INFO.EQ.O .AND. IINFO.GT.O )
  $
            INFO = IINFO + J - 1
        DO 10 I = J, MIN(M, J+JB-1)
            IPIV(I) = J - 1 + IPIV(I)
10
         CONTINUE
         CALL DLASWP( J-1, A, LDA, J, J+JB-1, IPIV, 1 )
        IF ( J+JB.LE.N ) THEN
            CALL DLASWP( N-J-JB+1, A( 1, J+JB ), LDA, J, J+JB-1,
  $
            CALL DTRSM( 'Left', 'Lower', 'No transpose', 'Unit', JB,
  $
                        N-J-JB+1, ONE, A(J, J), LDA, A(J, J+JB),
                        LDA )
               CALL DGEMM ( 'No transpose', 'No transpose', M-J-JB+1,
  $
                           N-J-JB+1, JB, -ONE, A(J+JB, J), LDA,
  $
                           A( J, J+JB ), LDA, ONE, A( J+JB, J+JB ),
                           LDA )
            END IF
         END IF
20
      CONTINUE
```

# LAPACK LU factorization with partial pivoting blocked algorithm (abbreviated)



```
DO 20 J = 1, MIN(M, N), NB
         JB = MIN(MIN(M, N) - J + 1, NB)
         CALL DGETF2( M-J+1, JB, A( J, J ), LDA, IPIV( J ), IINFO )
        IF( INFO.EQ.O .AND. IINFO.GT.O )
  $
            INFO = IINFO + J - 1
        DO 10 I = J, MIN(M, J+JB-1)
            IPIV(I) = J - 1 + IPIV(I)
10
         CONTINUE
         CALL DLASWP( J-1, A, LDA, J, J+JB-1, IPIV, 1 )
        IF ( J+JB.LE.N ) THEN
            CALL DLASWP( N-J-JB+1, A( 1, J+JB ), LDA, J, J+JB-1,
  $
                         IPIV, 1)
            CALL DTRSM( 'Left', 'Lower', 'No transpose', 'Unit', JB,
  $
                        N-J-JB+1, ONE, A(J, J), LDA, A(J, J+JB),
  $
                        LDA )
               CALL DGEMM ( 'No transpose', 'No transpose', M-J-JB+1,
 $
                           N-J-JB+1, JB, -ONE, A(J+JB, J), LDA,
  $
                           A( J, J+JB ), LDA, ONE, A( J+JB, J+JB ),
                           T-DA )
            END IF
         END IF
      CONTINUE
```

## Performance (Intel Xeon 3.4GHz)



June 19,

# **Evolving Beyond?**

- New architectures with many "cores"
  - Symmetric Multi-Processors (SMPs)
  - Multicore architectures

 Algorithms encoded in LAPACK don't always parallelize well

### AMD Opteron 8 cores (2.4GHz)

Cholesky (lower) performance with various libraries (m = p) ACML 3.60 GotoBLAS 1.09 APACK 3.0 + GotoBLAS 1.09 FLAME + GotoBLAS 1.09 FLAME + LAPACK 3.0 + GotoBLAS 1.09 GFLOPS problem size p

e/

Jι

# Evolution vs Intelligent Design

- LAPACK code is hard to write/read/maintain/alter
- Formal Linear Algebra Methods Environment (FLAME) Project
  - Based on insights from the PLAPACK project
  - Started around 2000. First official library release (libFLAME 1.0): April 1, 2007
  - Collaboration between UT Dept. of Computer Sciences, TACC, and UJI-Spain
  - Systematic approach to deriving, presenting, and implementing algorithms

## Why the FLAME API?

From the "LAPACK 3.1.1. changes" log:

```
replaced calls of the form

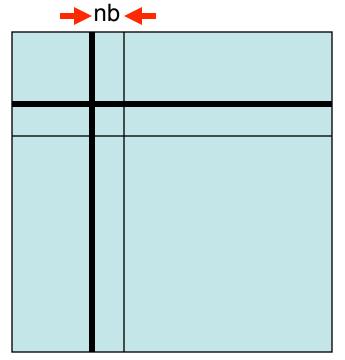
CALL SCOPY( N, WORK, 1, TAU, 1 )

with

CALL SCOPY( N-1, WORK, 1, TAU, 1 )

at line 694 for s/dchkhs and line 698 for c/zchkhs.

(TAU is only of length N-1.)
```



June 19, 2008

Algorithm: 
$$[A] := LU_BLK_VAR5(A)$$

Partition 
$$A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$
  
where  $A_{TL}$  is  $0 \times 0$ 

while  $m(A_{TL}) < m(A)$  do

Determine block size bRepartition

$$\begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{pmatrix}$$
where  $A_{11}$  is  $b \times b$ 

$$A_{11} = LU(A_{11})$$

$$A_{12} = TRILU(A_{11})^{-1}A_{12}$$

$$A_{21} = A_{21}TRIU(A_{11})^{-1}$$

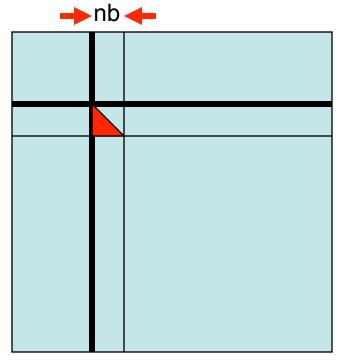
$$A_{22} = A_{22} - A_{21}A_{12}$$

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

endwhile

ORNL 08



June 19, 2008

Algorithm: 
$$[A] := LU_BLK_VAR5(A)$$

Partition 
$$A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$
  
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where  $A_{11}$  is  $b \times b$ 

$$A_{11} = \mathrm{LU}(A_{11})$$

$$A_{12} = \text{TRILU}(A_{11})^{-1} A_{12}$$

$$A_{21} = A_{21} \text{TRIU}(A_{11})^{-1}$$

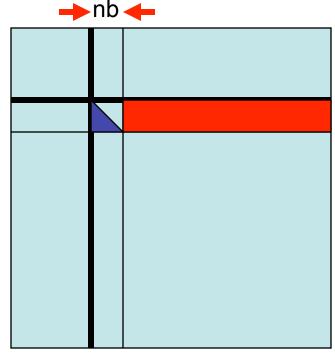
$$A_{22} = A_{22} - A_{21}A_{12}$$

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

endwhile

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June 19, 2008

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where  $A_{11}$  is  $b \times b$ 

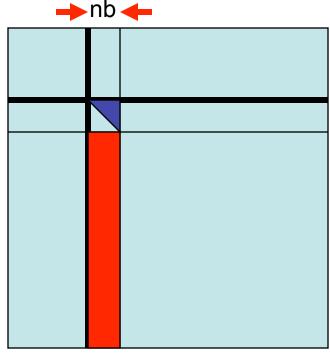
$$A_{11} = LU(A_{11})$$
  
 $A_{12} = TRILU(A_{11})^{-1}A_{12}$   
 $A_{21} = A_{21}TRIU(A_{11})^{-1}$   
 $A_{22} = A_{22} - A_{21}A_{12}$ 

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

endwhile

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June 19, 2008

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where  $A_{11}$  is  $b \times b$ 

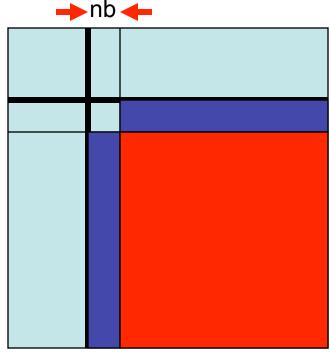
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 $A_{12} = TRILU(A_{11})^{-1}A_{12}$   
 $A_{21} = A_{21}TRIU(A_{11})^{-1}$   
 $A_{22} = A_{22} - A_{21}A_{12}$ 

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

endwhile

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June 19, 2008

**Algorithm:** 
$$[A] := LU_BLK_VAR5(A)$$

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$$A_{11} = \mathrm{LU}(A_{11})$$

$$A_{12} = \text{Trilu}(A_{11})^{-1}A_{12}$$

$$A_{21} = A_{21} \text{TRIU}(A_{11})^{-1}$$

$$A_{22} = A_{22} - A_{21}A_{12}$$

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

endwhile

ORNL 08

Partition 
$$A \to \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$

where  $A_{TL}$  is  $0 \times 0$ while  $m(A_{TL}) < m(A)$  do

Determine block size b Repartition

$$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{pmatrix}$$
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$$A_{12} = \text{TRILU}(A_{11})^{-1}A_{12}$$

$$A_{21} = A_{21} \text{TRIU}(A_{11})^{-1}$$

$$A_{22} = A_{22} - A_{21}A_{12}$$

#### Continue with

$$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{pmatrix}$$

```
FLA Part 2x2( A,
                  &ATL, &ATR,
                   &ABL, &ABR,
                                  0, 0, FLA TL );
 while (FLA Obj length( ATL ) < FLA Obj length( A )){</pre>
  b = min(FLA Obj length(ABR), nb alg);
   FLA Repart 2x2 to 3x3
     ( ATL, /**/ ATR,
                        &A00, /**/ &A01, &A02,
    &A10, /**/ &A11, &A12,
       ABL, /**/ ABR,
                           &A20, /**/ &A21, &A22,
       b, b, FLA_BR );
  LU unb var5( A11 );
   FLA Trsm( FLA LEFT, FLA LOWER TRIANGULAR,
            FLA NO TRANSPOSE, FLA UNIT DIAG,
            FLA ONE, A11, A12);
  FLA Trsm( FLA RIGHT, FLA UPPER TRIANGULAR,
            FLA NO TRANSPOSE, FLA NONUNIT DIAG,
            FLA ONE, A11, A21);
   FLA Gemm ( FLA NO TRANSPOSE, FLA NO TRANSPOSE,
           FLA_MINUS_ONE, A21, A12, FLA_ONE, A22 );
   FLA_Cont_with_3x3_to_2x2
     ( &ATL, /**/ &ATR, A00, A01, /**/ A02,
                            A10, A11, /**/ A12,
     /* ********* */ /* *********** */
       &ABL, /**/ &ABR, A20, A21, /**/ A22,
       FLA TL );
 }
```

Partition 
$$A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$

where  $A_{TL}$  is  $0 \times 0$ while  $m(A_{TL}) < m(A)$  do

Determine block size bRepartition

$$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{pmatrix}$$
where  $A_{11}$  is  $b \times b$ 

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$$A_{21} = A_{21} \text{TRIU}(A_{11})^{-1}$$

$$A_{22} = A_{22} - A_{21}A_{12}$$

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

```
FLA Part 2x2( A,
                   &ATL, &ATR,
                    &ABL, &ABR,
                                    0, 0, FLA TL );
while (FLA Obj length( ATL ) < FLA Obj length( A )) {</pre>
  b = min( FLA Obj length( ABR ), nb alg );
   FLA Repart 2x2 to 3x3
     ( ATL, /**/ ATR,
                         &A00, /**/ &A01, &A02,
    /* ******** */ /* ************** */
                            &A10, /**/ &A11, &A12,
                            &A20, /**/ &A21, &A22,
       ABL, /**/ ABR,
       b, b, FLA_BR );
  LU unb var5( A11 );
   FLA Trsm( FLA LEFT, FLA LOWER TRIANGULAR,
            FLA NO TRANSPOSE, FLA UNIT DIAG,
            FLA ONE, A11, A12);
  FLA Trsm( FLA RIGHT, FLA UPPER TRIANGULAR,
            FLA NO TRANSPOSE, FLA NONUNIT DIAG,
            FLA ONE, A11, A21);
   FLA Gemm ( FLA NO TRANSPOSE, FLA NO TRANSPOSE,
            FLA_MINUS_ONE, A21, A12, FLA_ONE, A22 );
   FLA_Cont_with_3x3_to_2x2
     ( &ATL, /**/ &ATR, A00, A01, /**/ A02,
                              A10, A11, /**/ A12,
     /* ********* */ /* *********** */
       &ABL, /**/ &ABR, A20, A21, /**/ A22,
       FLA TL );
}
```

Partition 
$$A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$
  
where  $A_{TL}$  is  $0 \times 0$ 

while  $m(A_{TL}) < m(A)$  do

Determine block size b

#### Repartition

$$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{pmatrix}$$
where  $A_{11}$  is  $b \times b$ 

$$A_{11} = LU(A_{11})$$

$$A_{12} = TRILU(A_{11})^{-1}A_{12}$$

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#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
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\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
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A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

```
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                    &ABL, &ABR,
                                   0, 0, FLA TL );
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  b = min(FLA Obj length(ABR), nb alg);
   FLA Repart 2x2 to 3x3
     &A00, /**/ &A01, &A02,
    /* ********** */
                           &A10, /**/ &A11, &A12,
       ABL, /**/ ABR,
                           &A20, /**/ &A21, &A22,
       b, b, FLA BR );
  LU unb var5( A11 );
   FLA Trsm( FLA LEFT, FLA LOWER TRIANGULAR,
            FLA NO TRANSPOSE, FLA UNIT DIAG,
            FLA ONE, A11, A12);
   FLA Trsm( FLA RIGHT, FLA UPPER TRIANGULAR,
            FLA NO TRANSPOSE, FLA NONUNIT DIAG,
            FLA ONE, A11, A21);
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   FLA_Cont_with_3x3_to_2x2
     A00, A01, /**/ A02,
                             A10, A11, /**/ A12,
     /* ********* */ /* ************ */
       &ABL, /**/ &ABR, A20, A21, /**/ A22,
       FLA TL );
 }
```

Partition 
$$A \to \begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix}$$

where  $A_{TL}$  is  $0 \times 0$ while  $m(A_{TL}) < m(A)$  do

Determine block size b Repartition

$$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{pmatrix}$$
where  $A_{11}$  is  $b \times b$ 

$$A_{11} = \mathrm{LU}(A_{11})$$

$$A_{12} = \text{TRILU}(A_{11})^{-1}A_{12}$$

$$A_{21} = A_{21} \text{TRIU}(A_{11})^{-1}$$

$$A_{22} = A_{22} - A_{21}A_{12}$$

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

```
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  b = min( FLA Obj length( ABR ), nb alg );
  FLA Repart 2x2 to 3x3
     ( ATL, /**/ ATR,
                        &A00, /**/ &A01, &A02,
    &A10, /**/ &A11, &A12,
                          &A20, /**/ &A21, &A22,
       ABL, /**/ ABR,
       b, b, FLA_BR );
  LU unb var5( A11 );
  FLA Trsm( FLA LEFT, FLA LOWER TRIANGULAR,
           FLA NO TRANSPOSE, FLA UNIT DIAG,
           FLA ONE, A11, A12);
  FLA Trsm( FLA RIGHT, FLA UPPER TRIANGULAR,
            FLA NO TRANSPOSE, FLA NONUNIT DIAG,
           FLA ONE, A11, A21 );
  FLA Gemm ( FLA NO TRANSPOSE, FLA NO TRANSPOSE,
           FLA MINUS ONE, A21, A12, FLA ONE, A22 );
  FLA Cont with 3x3 to 2x2
     A00, A01, /**/ A02,
                            A10, A11, /**/ A12,
     /* ********* */ /* ************ */
       &ABL, /**/ &ABR,
                            A20, A21, /**/ A22,
       FLA TL );
```

Partition 
$$A \to \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$

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where  $A_{11}$  is  $b \times b$ 

$$A_{11} = LU(A_{11})$$
  
 $A_{12} = TRILU(A_{11})^{-1}A$ 

 $A_{12} = \text{TRILU}(A_{11})^{-1} A_{12}$   $A_{21} = A_{21} \text{TRIU}(A_{11})^{-1}$ 

 $A_{22} = A_{22} - A_{21}A_{12}$ 

#### Continue with

$$\left(\begin{array}{c|c|c}
A_{TL} & A_{TR} \\
\hline
A_{BL} & A_{BR}
\end{array}\right) \leftarrow \left(\begin{array}{c|c|c}
A_{00} & A_{01} & A_{02} \\
\hline
A_{10} & A_{11} & A_{12} \\
\hline
A_{20} & A_{21} & A_{22}
\end{array}\right)$$

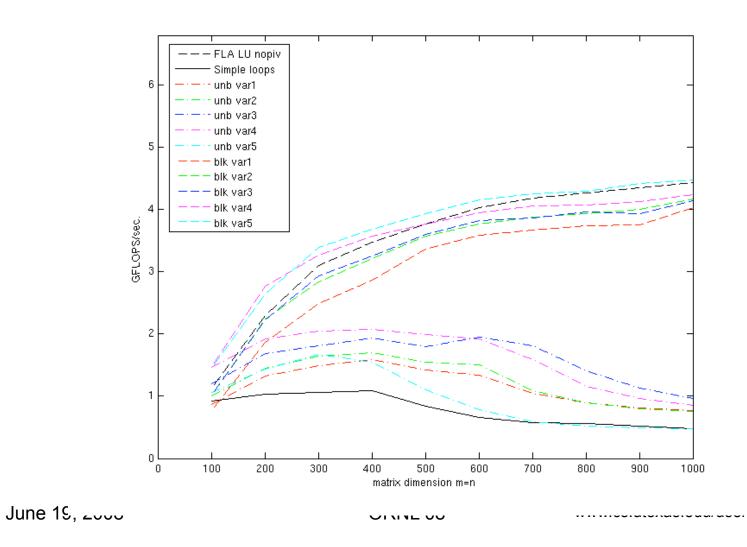
```
FLA Part 2x2(A,
                  &ATL, &ATR,
                   &ABL, &ABR,
                                 0, 0, FLA TL );
 while (FLA Obj length( ATL ) < FLA Obj length( A )){</pre>
  b = min( FLA Obj length( ABR ), nb alg );
  FLA Repart 2x2 to 3x3
     &A00, /**/ &A01, &A02,
    /* ********* */
                          &A10, /**/ &A11, &A12,
       ABL, /**/ ABR,
                          &A20, /**/ &A21, &A22,
       b, b, FLA BR );
  LU unb var5( A11 );
  FLA_Trsm( FLA_LEFT, FLA_LOWER TRIANGULAR,
           FLA NO TRANSPOSE, FLA UNIT DIAG,
           FLA ONE, A11, A12);
  FLA Trsm (FLA RIGHT, FLA UPPER TRIANGULAR,
            FLA NO TRANSPOSE, FLA NONUNIT DIAG,
           FLA ONE, A11, A21);
  FLA Gemm ( FLA NO TRANSPOSE, FLA NO TRANSPOSE,
           FLA MINUS ONE, A21, A12, FLA ONE, A22);
   /*----*/
   FLA Cont with 3x3 to 2x2
     ( &ATL, /**/ &ATR,
                           A00, A01, /**/ A02,
                            A10, A11, /**/ A12,
     /* ********* */ /* *********** */
       &ABL, /**/ &ABR, A20, A21, /**/ A22,
       FLA TL );
 }
```

# An algorithm for every occasion

- There are five loop-based algorithms for LU factorization without pivoting
  - Five unblocked
  - Five blocked

 On different architectures different algorithm will achieve best performance

## Performance (Intel Xeon 3.4GHz)

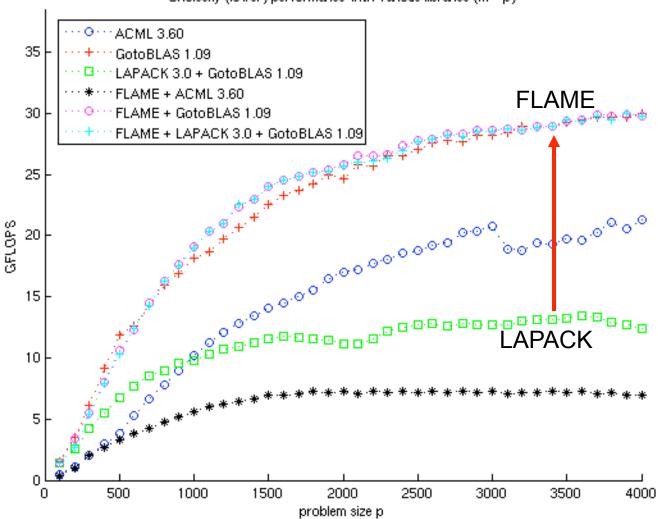


.'flame/

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### AMD Opteron 8 cores (2.4GHz)

Cholesky (lower) performance with various libraries (m = p)



e/

56

Jι

# Algorithms-by-Blocks

(some call these tiled algorithms)

- Distinguish
  - Blocked algorithms
  - Blocked algorithms that copy into contiguous blocks as an intermediate step
  - Algorithms-by-blocks (tiled algorithms)
- Fred Gustavson indicates he anticipated the need for algorithms-byblocks in 1986.
- First published use of storage by block: TR by Greg Henry, around 1992
- Many papers by Fred Gustavson, Bo Kagstrom and colleagues during late 1990s and beyond
- Many efforts to hide nastiness:
  - Skjellum et al, Wise, ...
- Application to OOC: SOLAR library by Toledo and Gustavson and POOCLAPACK from UT-Austin
- Our first effort: The FLASH extension of the FLAME/C API (FLAWN#12, 2004)
- Very recently: PLASMA project at UTK and SuperMatrix project at UT-Austin (2006-07)

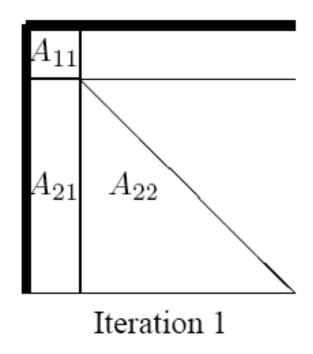
### The fundamental problem

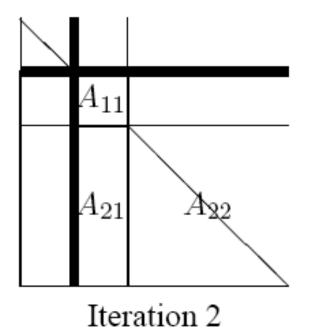
- People like Kazushige Goto optimize so well that it has been hard to show the benefits of storage by blocks.
- This changes with the emergence of multicore architectures(?).

### Overview

- A bit of history
- Programming algorithms-by-blocks is hard easy
  - An example: Cholesky factorization by blocks
- Programming algorithms-by-blocks further simplifies complicates programming (future) multicore architectures
- Conclusion
- Resources

# Example: Cholesky factorization





Algorithm: 
$$A := Chol_blk_var3(A)$$

Partition 
$$A \rightarrow \begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix}$$

where  $A_{TL}$  is  $0 \times 0$ while  $m(A_{TL}) < m(A)$  do

Determine block size bRepartition

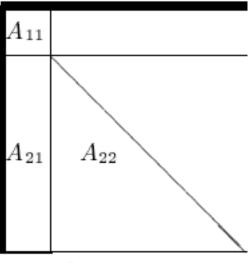
$$\begin{pmatrix} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{pmatrix} \rightarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ \hline A_{10} & A_{11} & A_{12} \\ \hline A_{20} & A_{21} & A_{22} \end{pmatrix}$$

where  $A_{11}$  is  $b \times b$ 

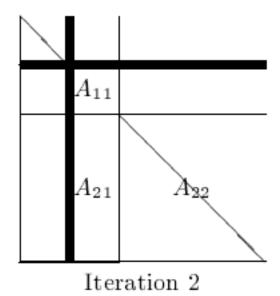
$$A_{11} = \text{Chol}(A_{11})$$
  
 $A_{21} = A_{21} \text{TRIL} (A_{11})^{-T}$   
 $A_{22} = A_{22} - \text{TRIL} (A_{21} A_{21}^T)$ 

#### Continue with

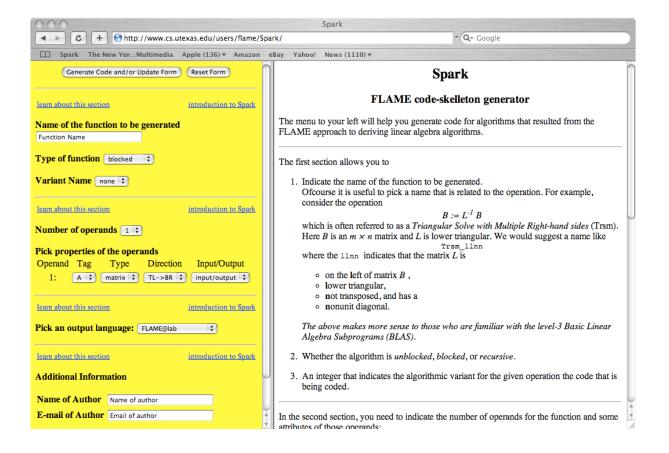
$$\begin{pmatrix} A_{TL} & A_{TR} \\ A_{BL} & A_{BR} \end{pmatrix} \leftarrow \begin{pmatrix} A_{00} & A_{01} & A_{02} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{pmatrix}$$

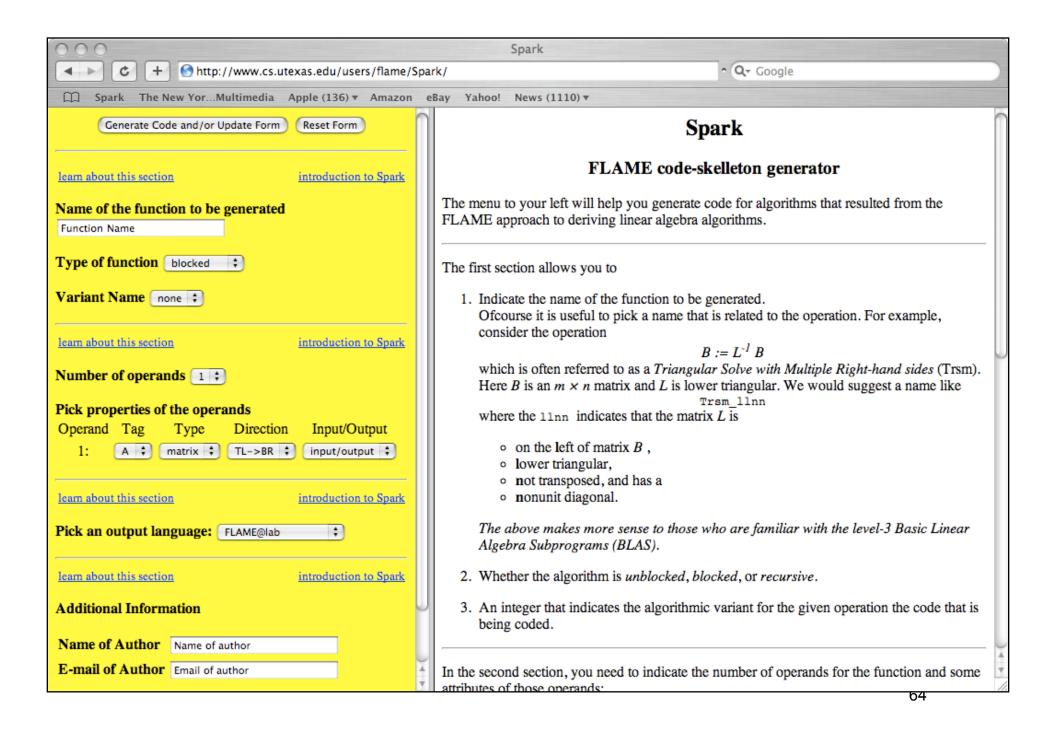


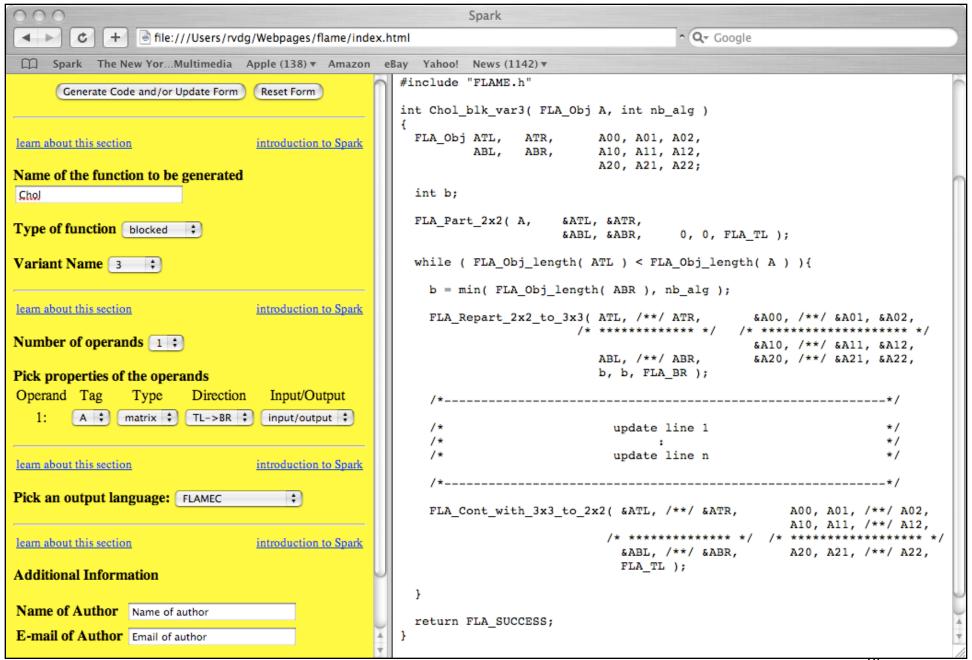
Iteration 1

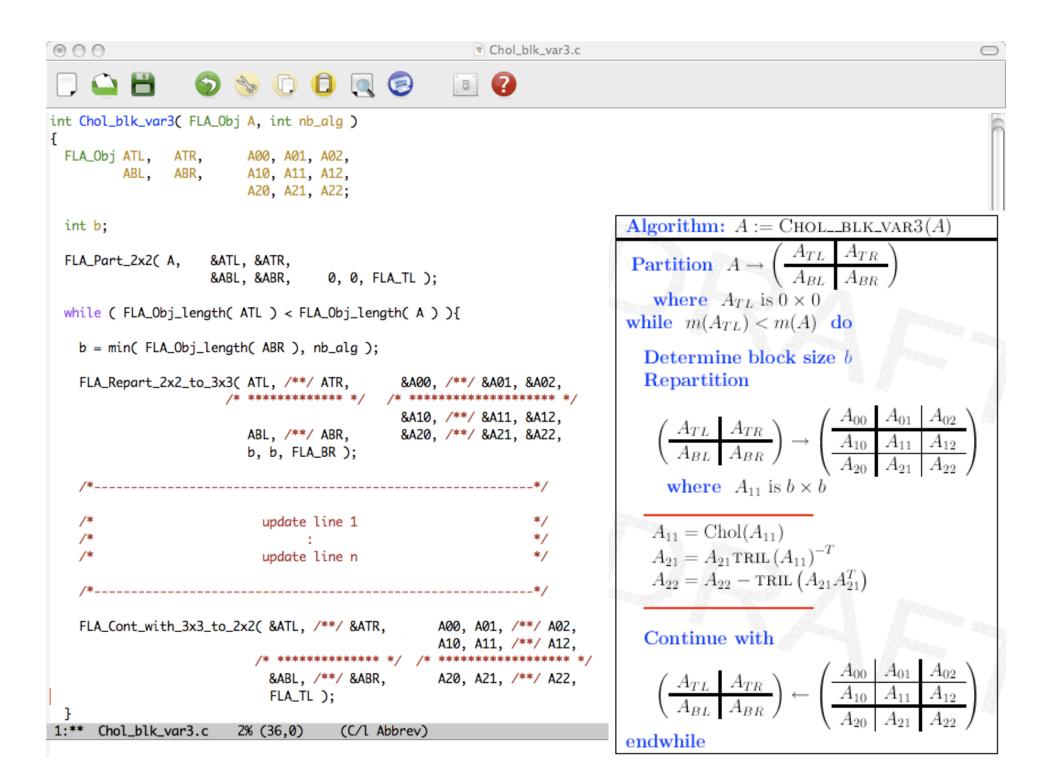


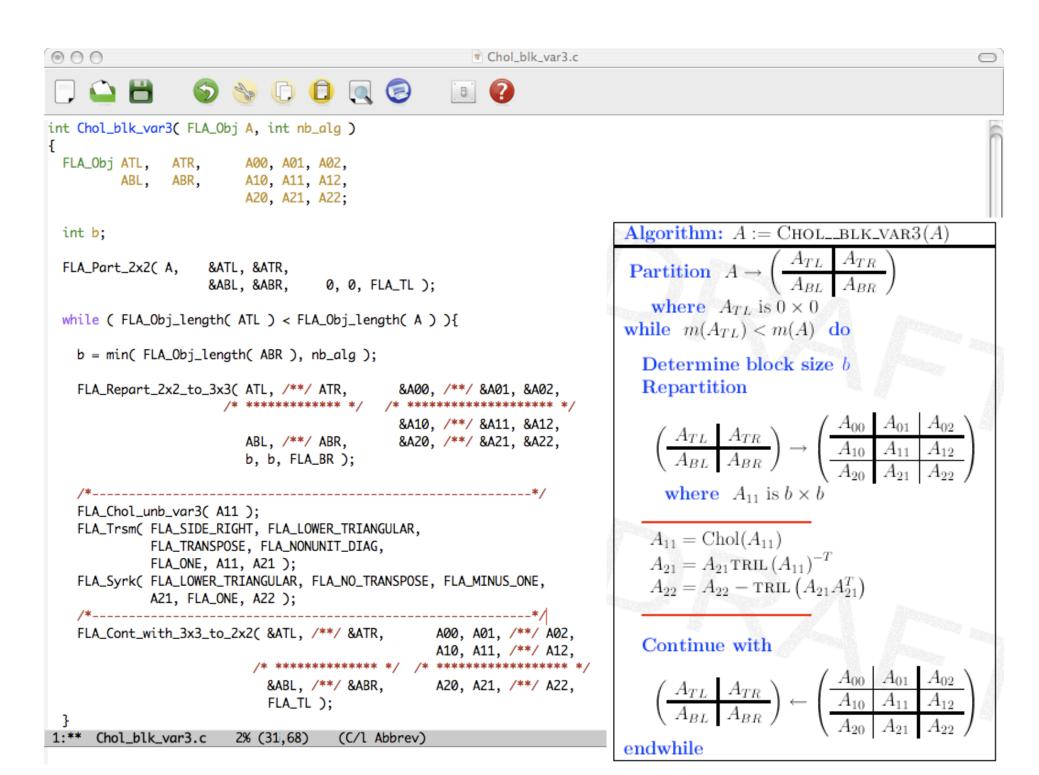
# Coding the Algorithm-by-Blocks in 15 minutes



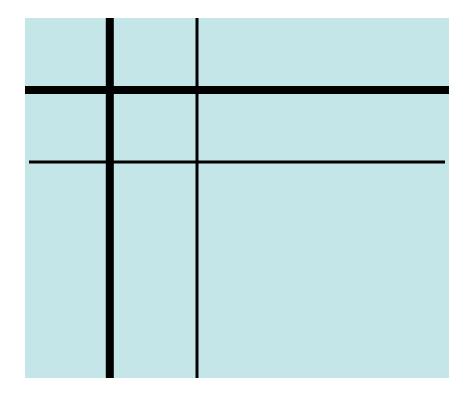




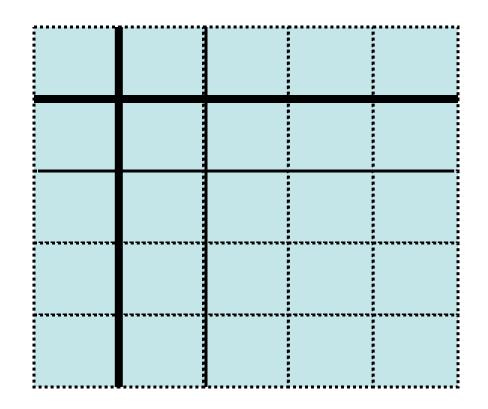




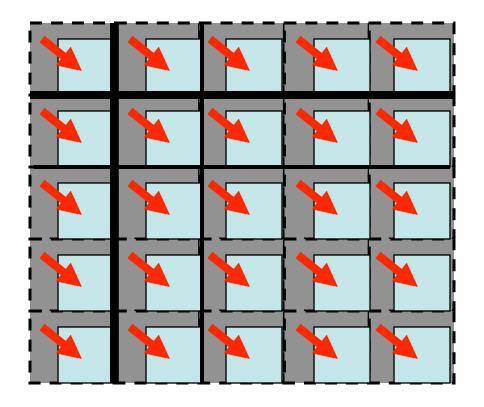
# **Blocked Algorithm**

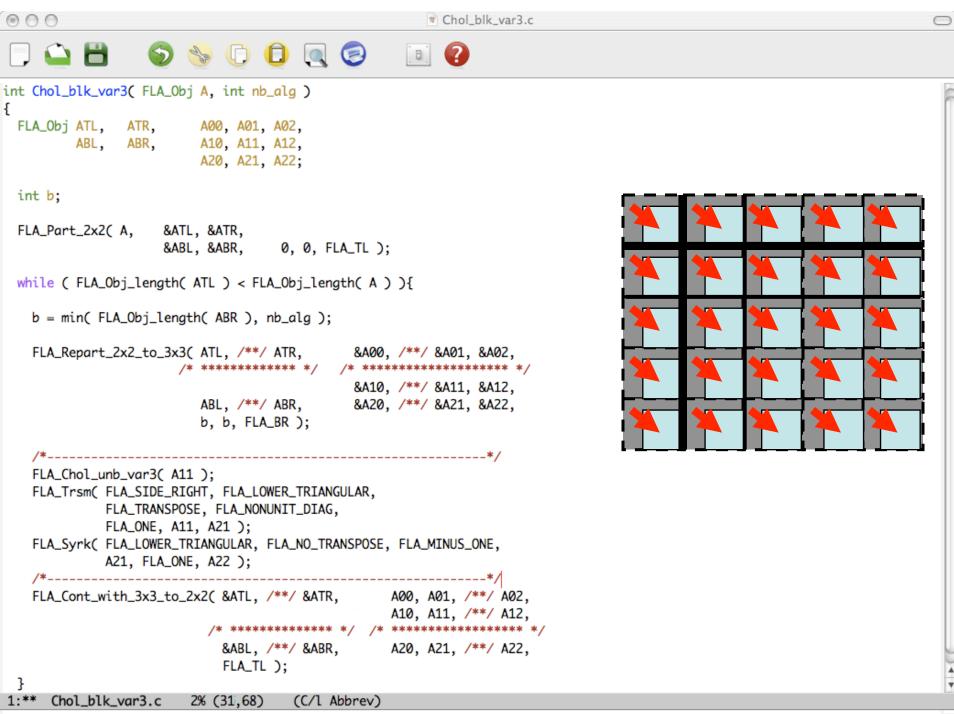


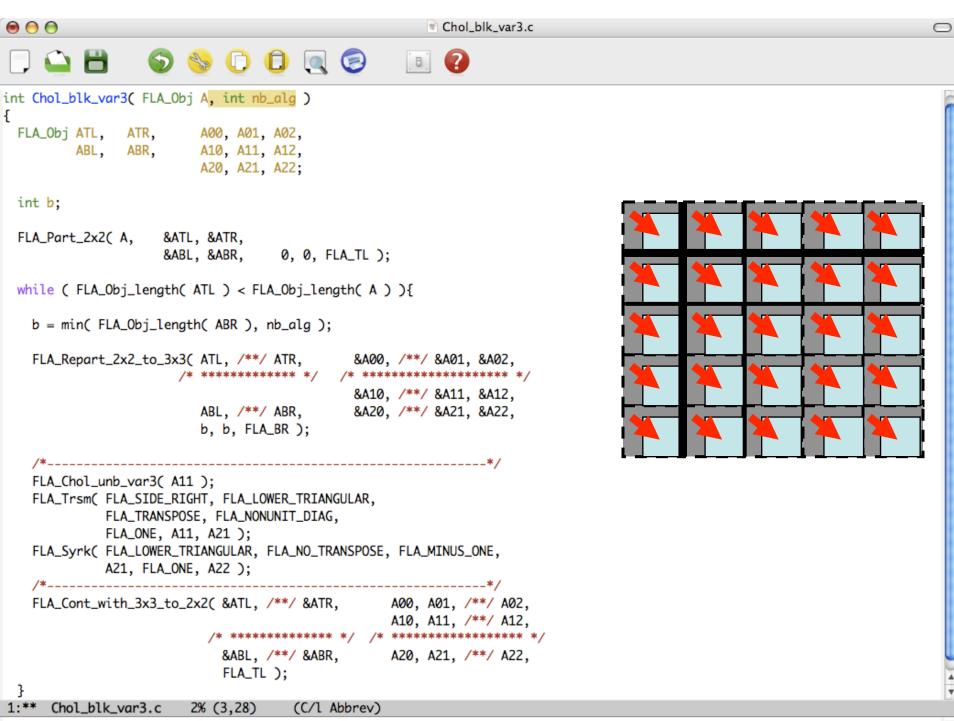
# Algorithm-by-Blocks

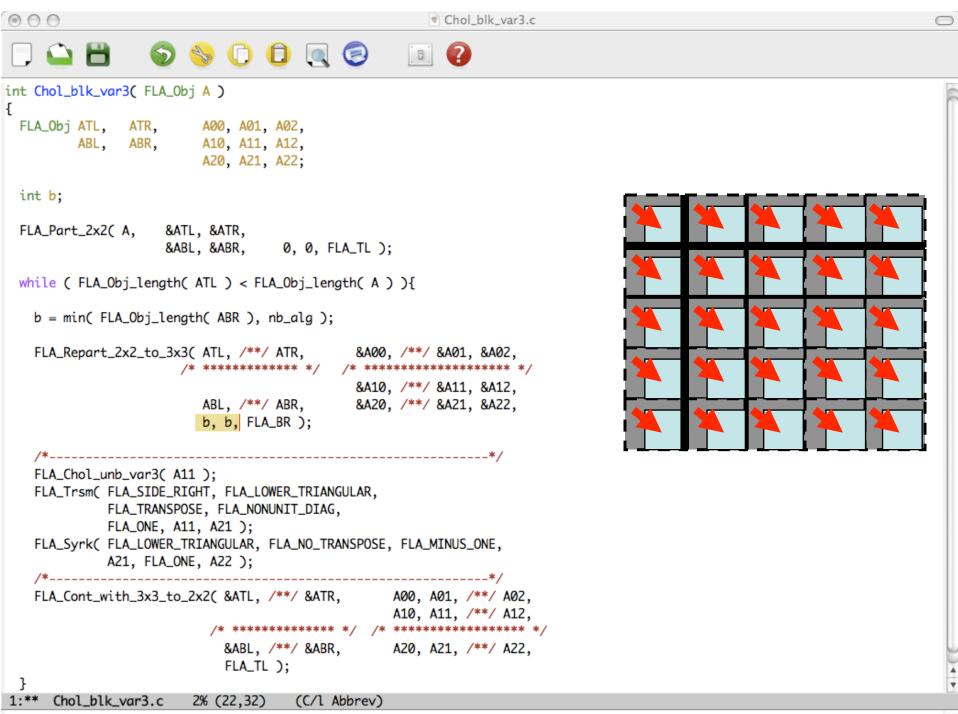


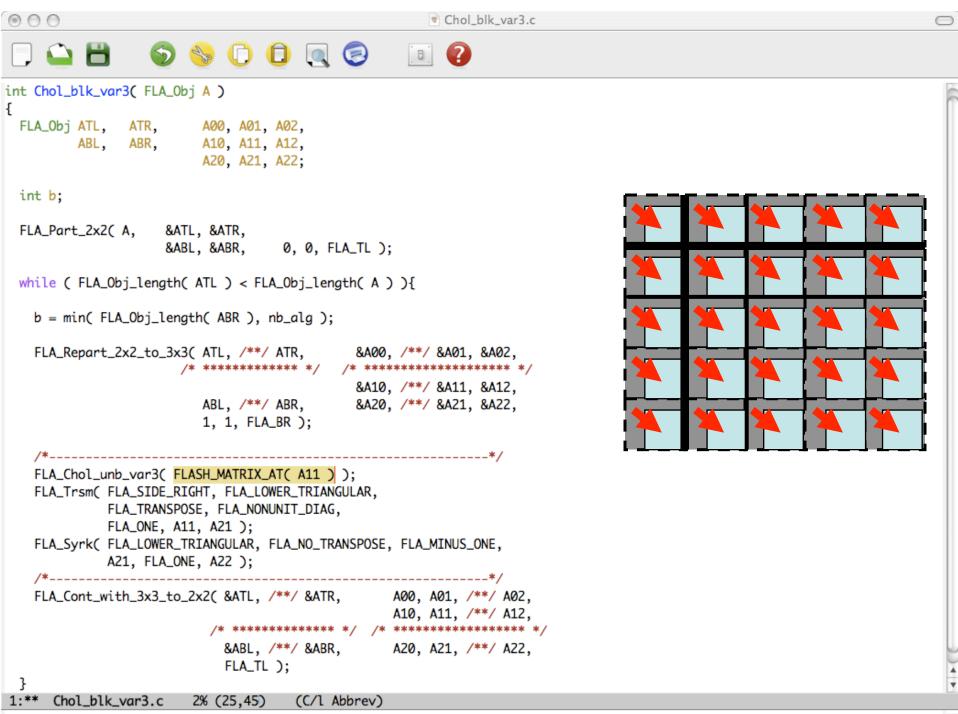
# Storage-by-Blocks

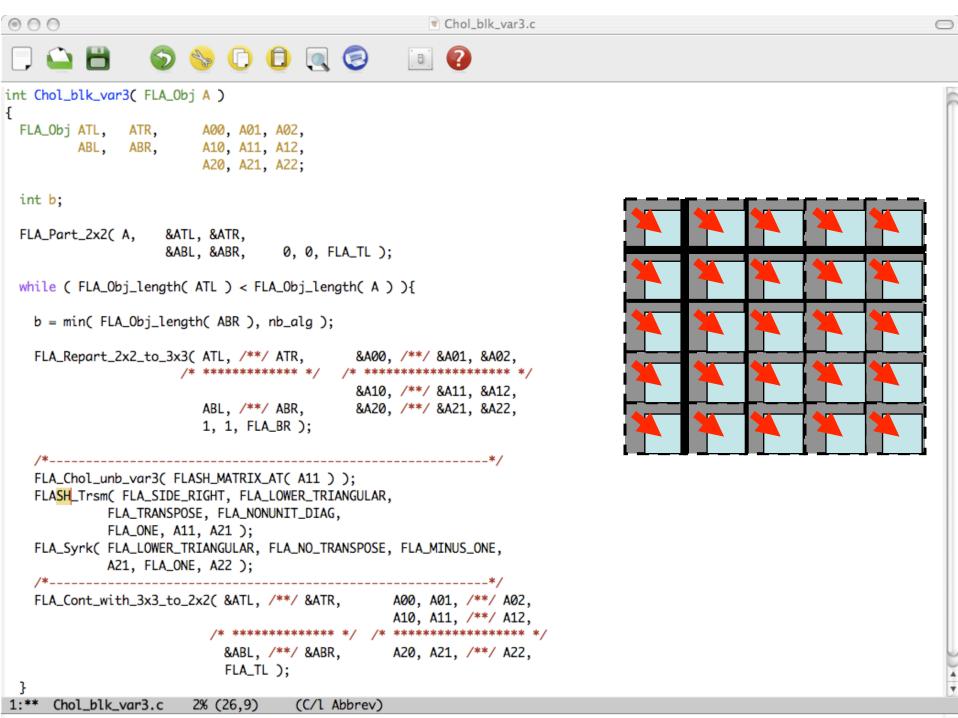


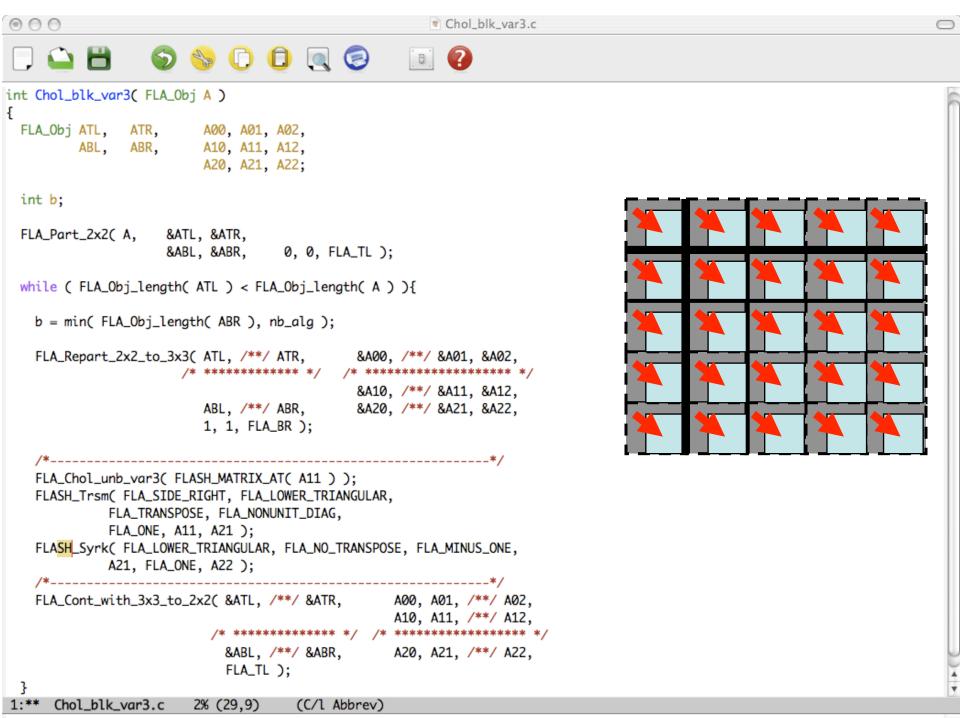


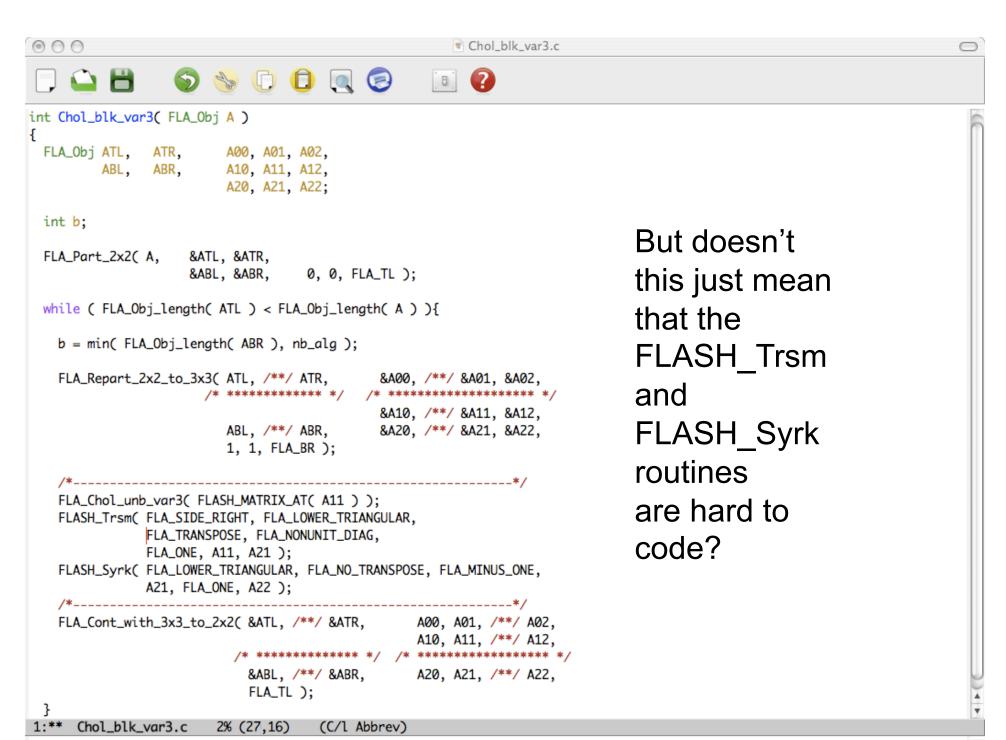


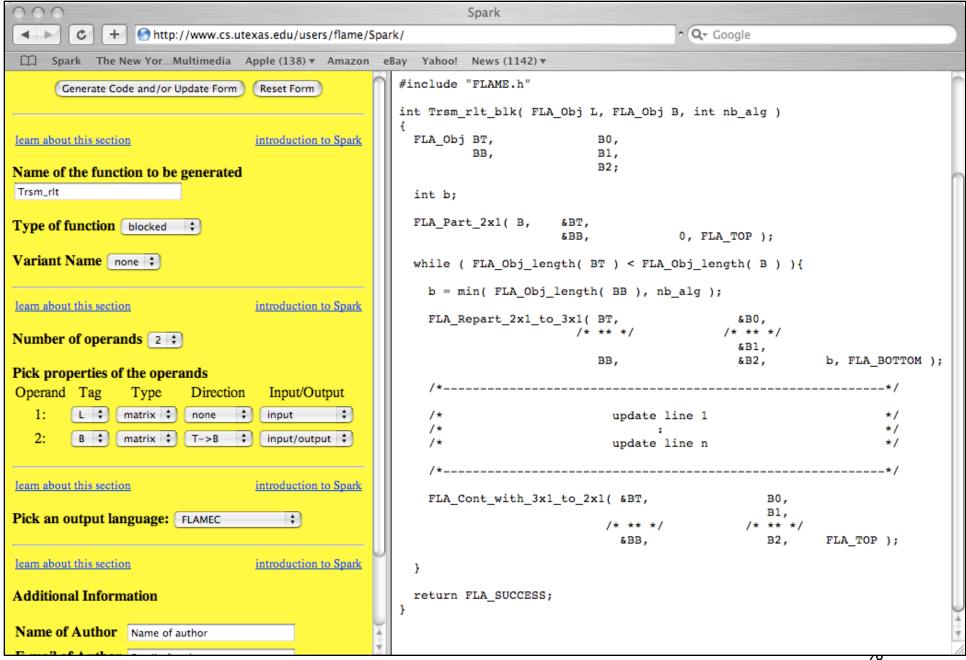


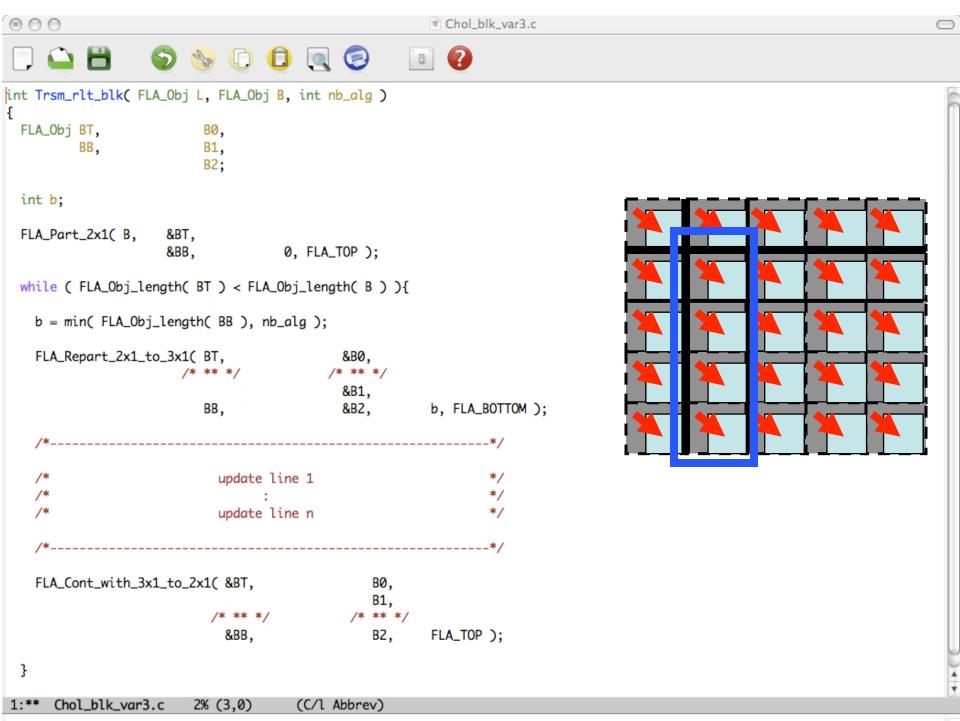


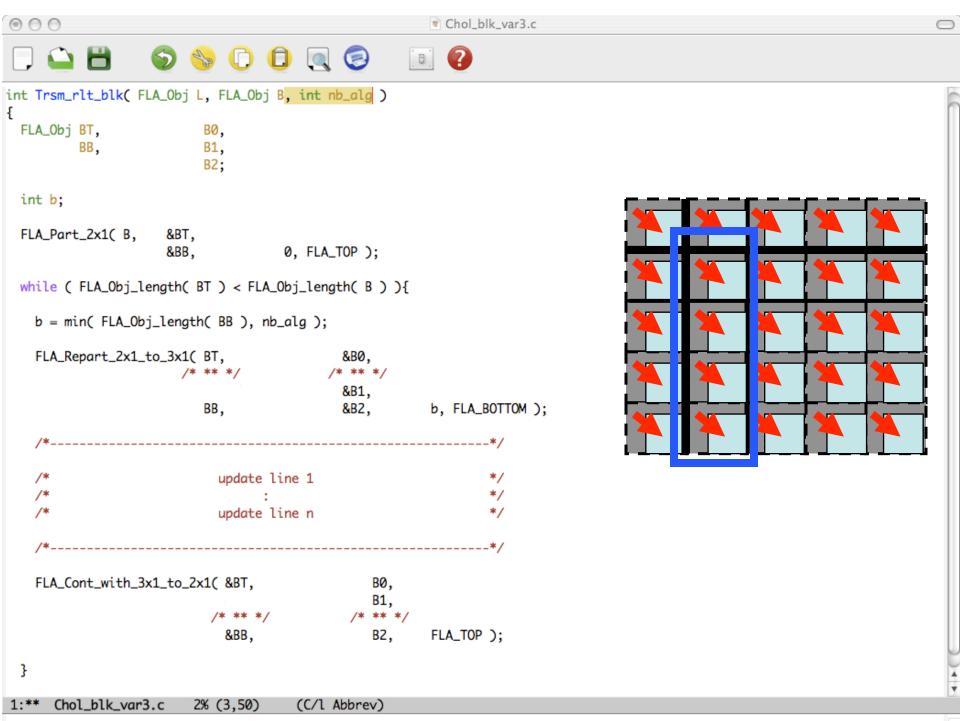


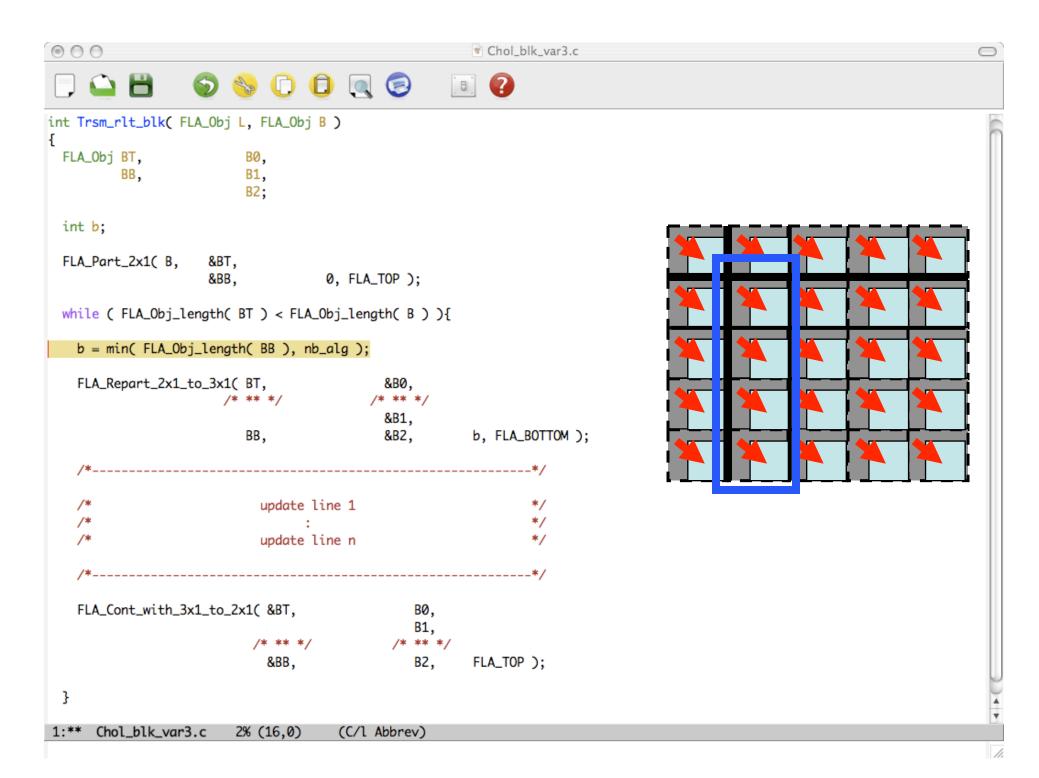


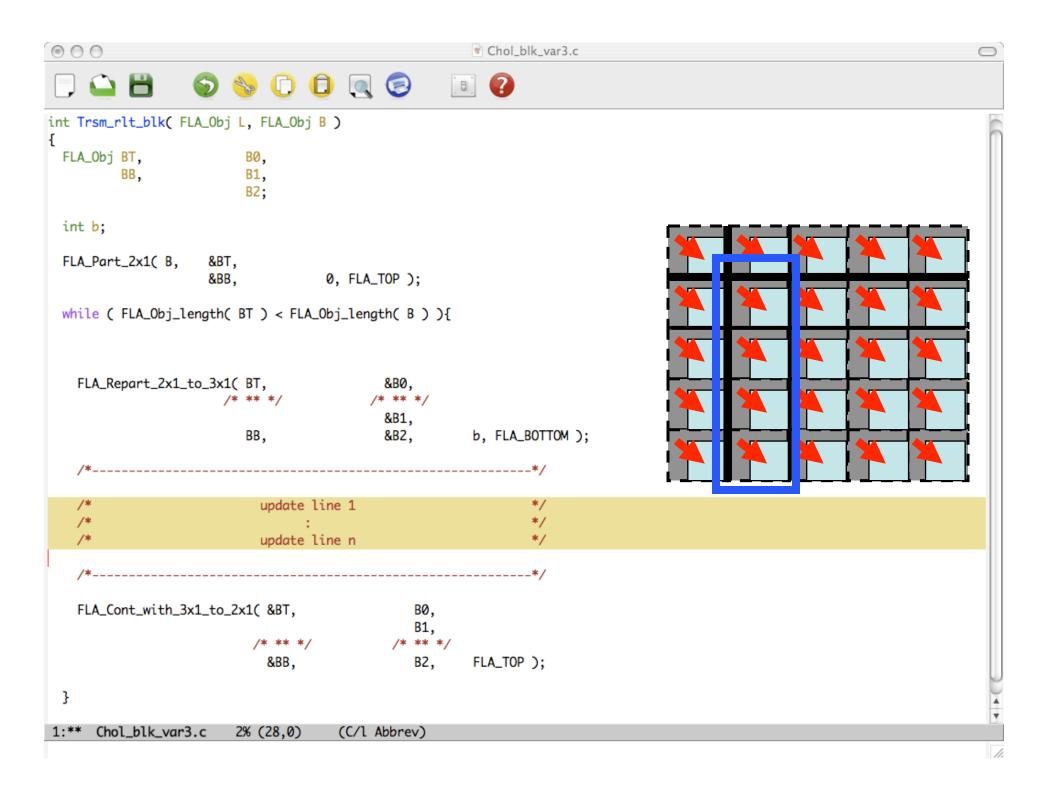


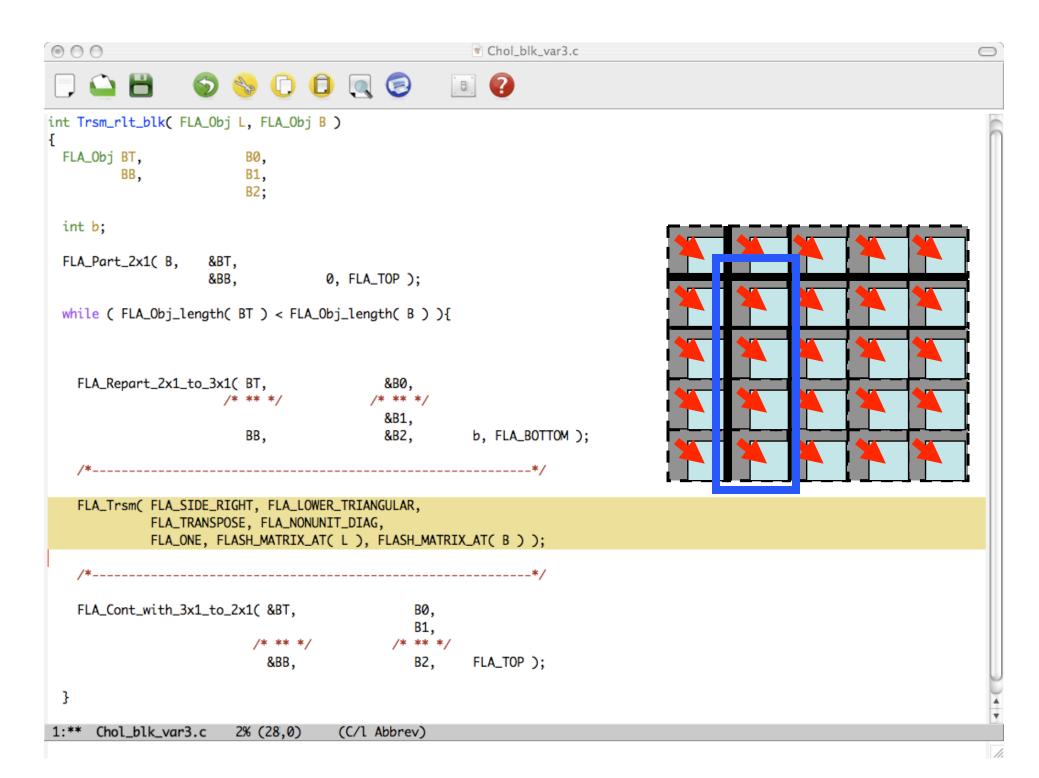


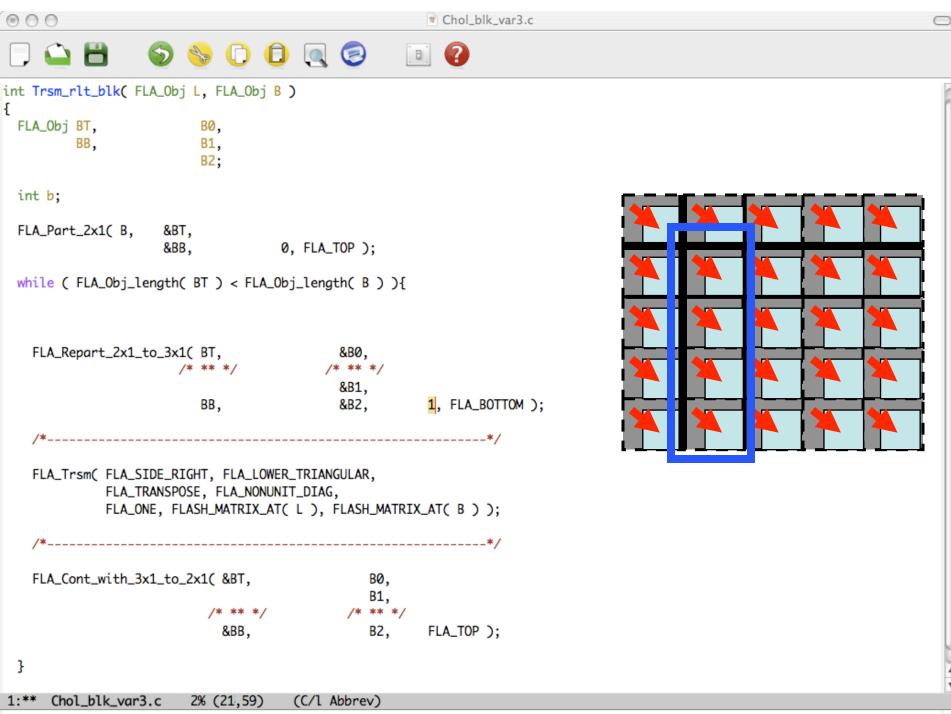


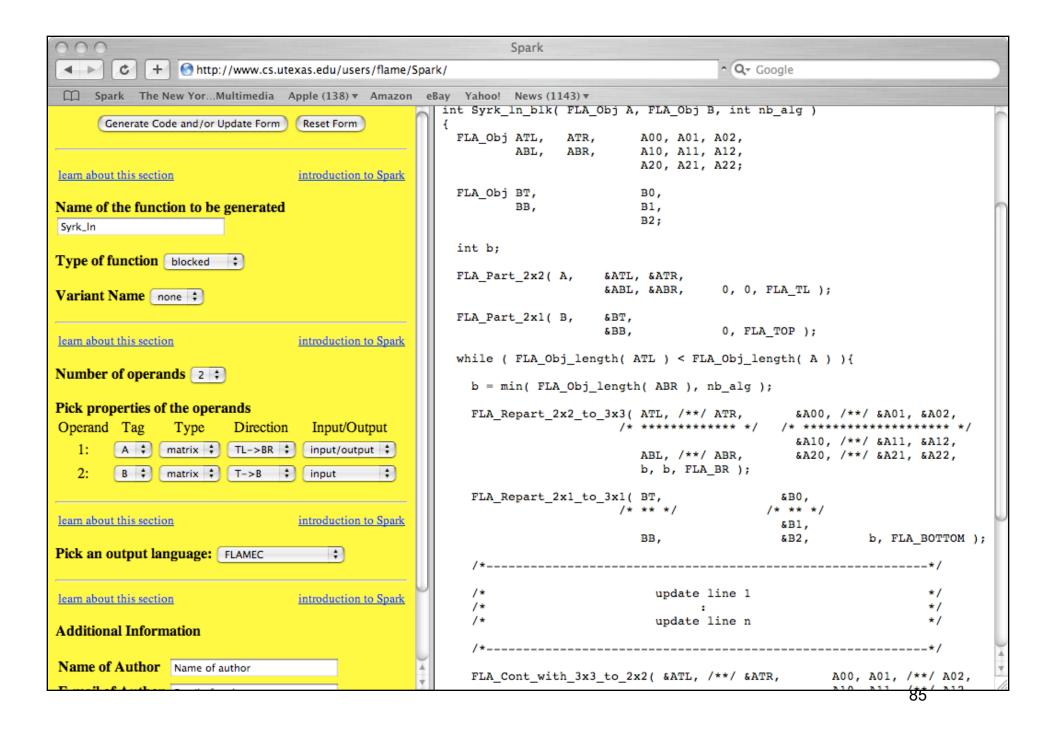


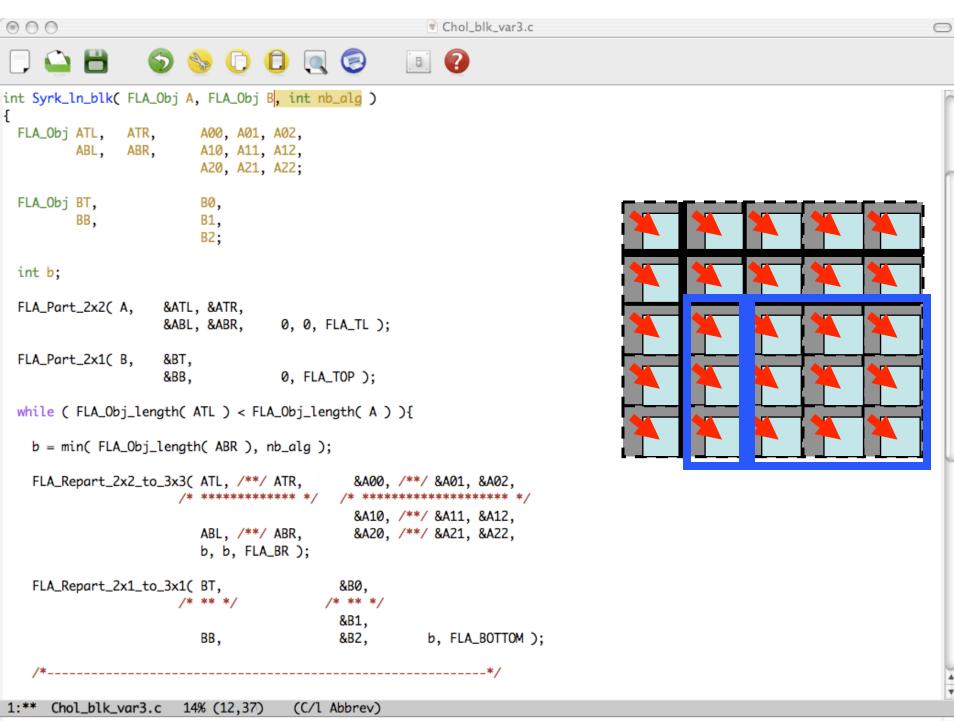


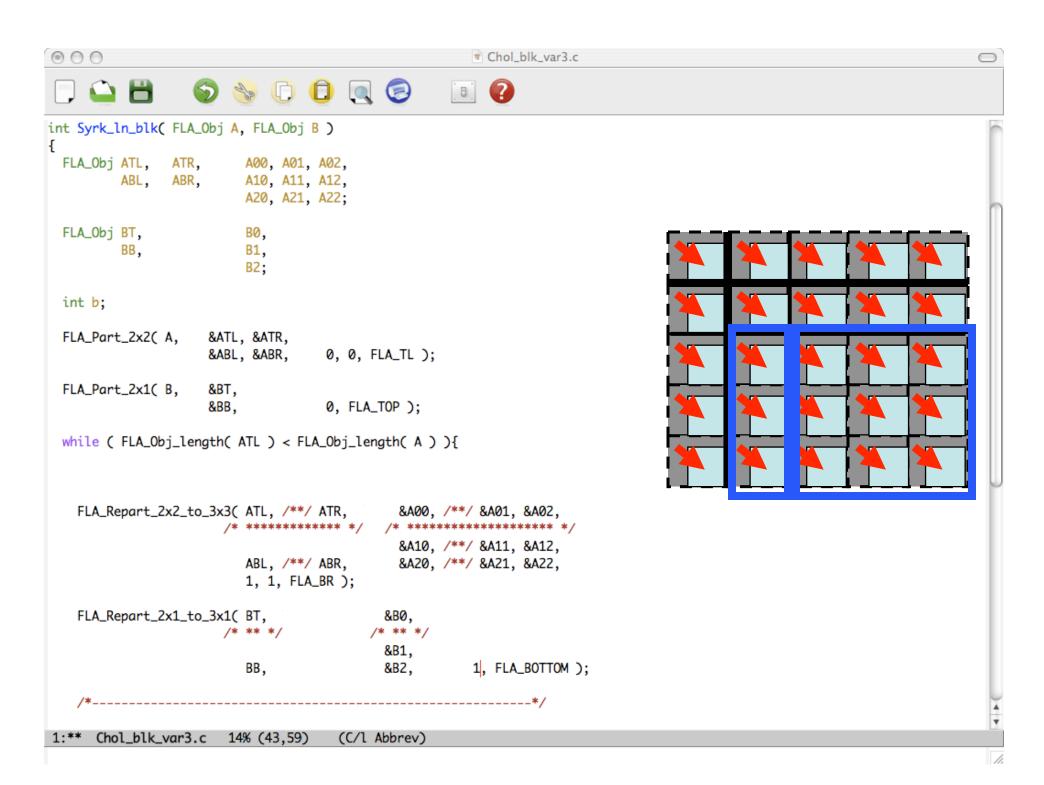


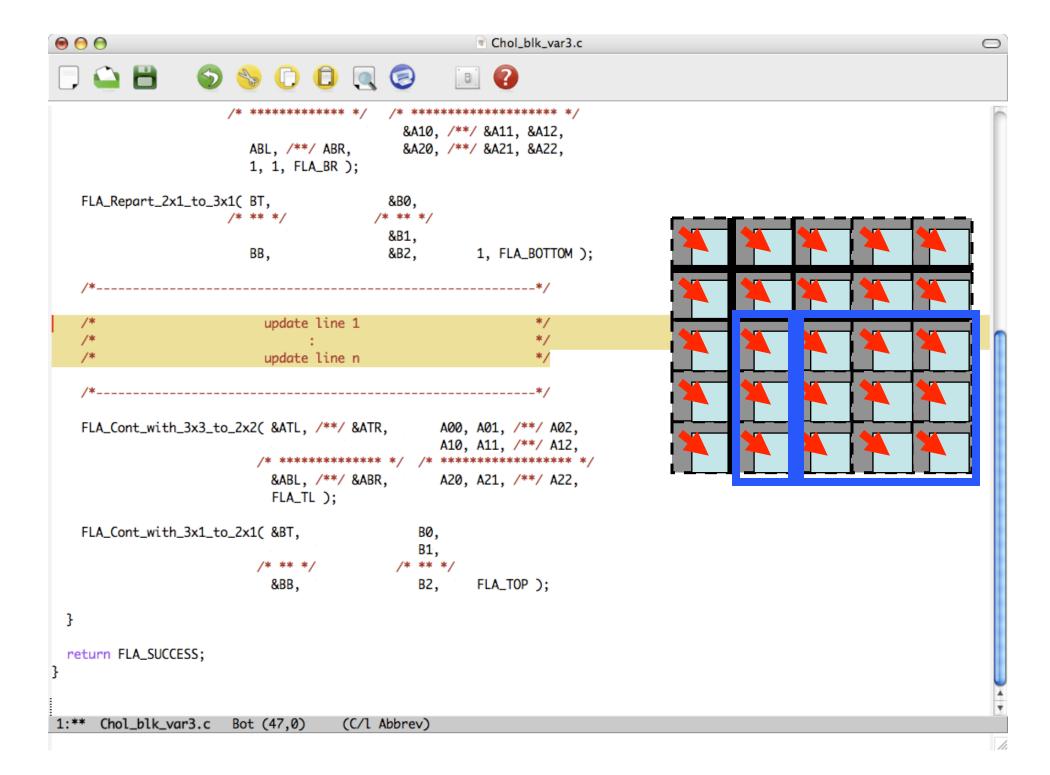


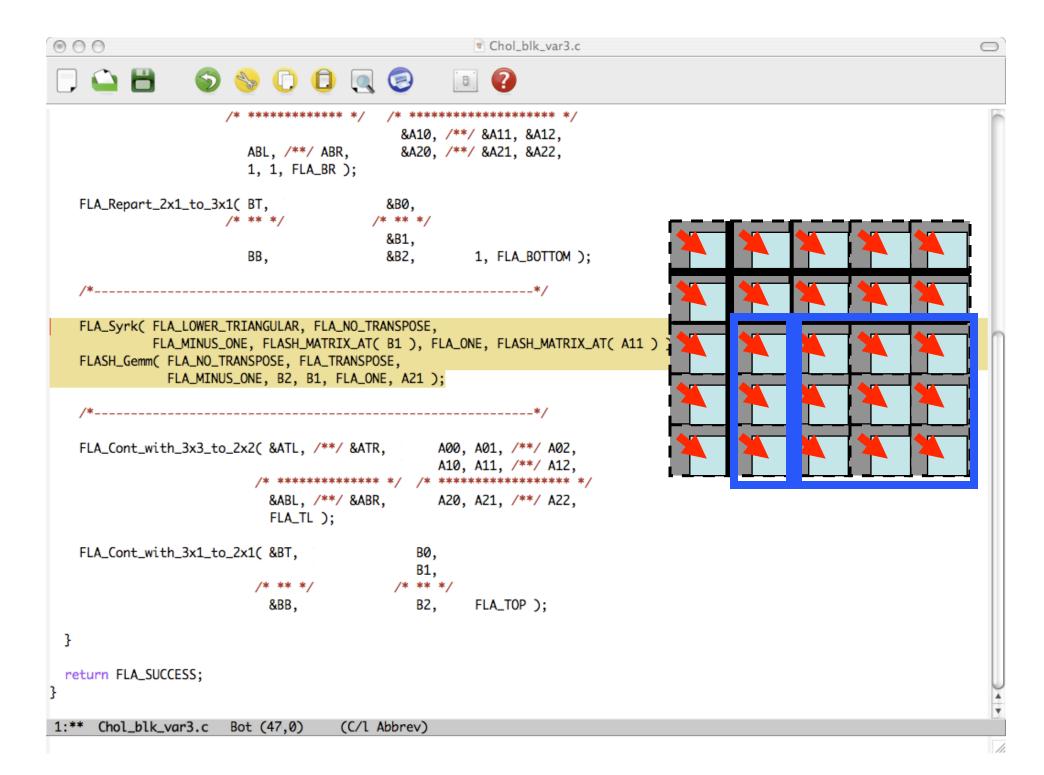


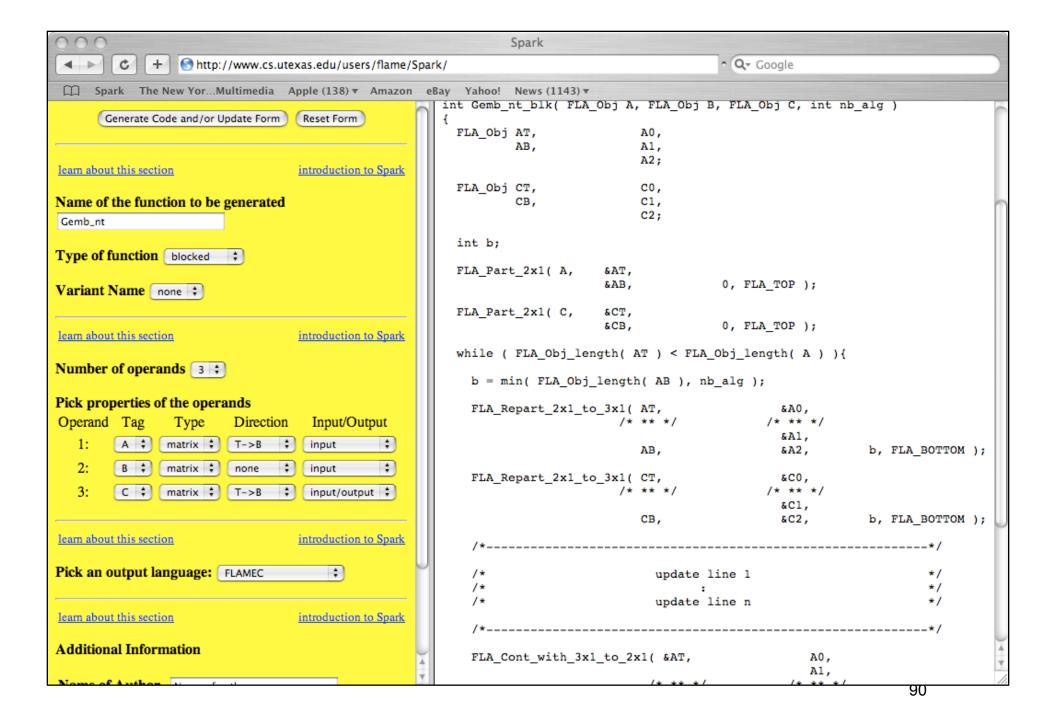




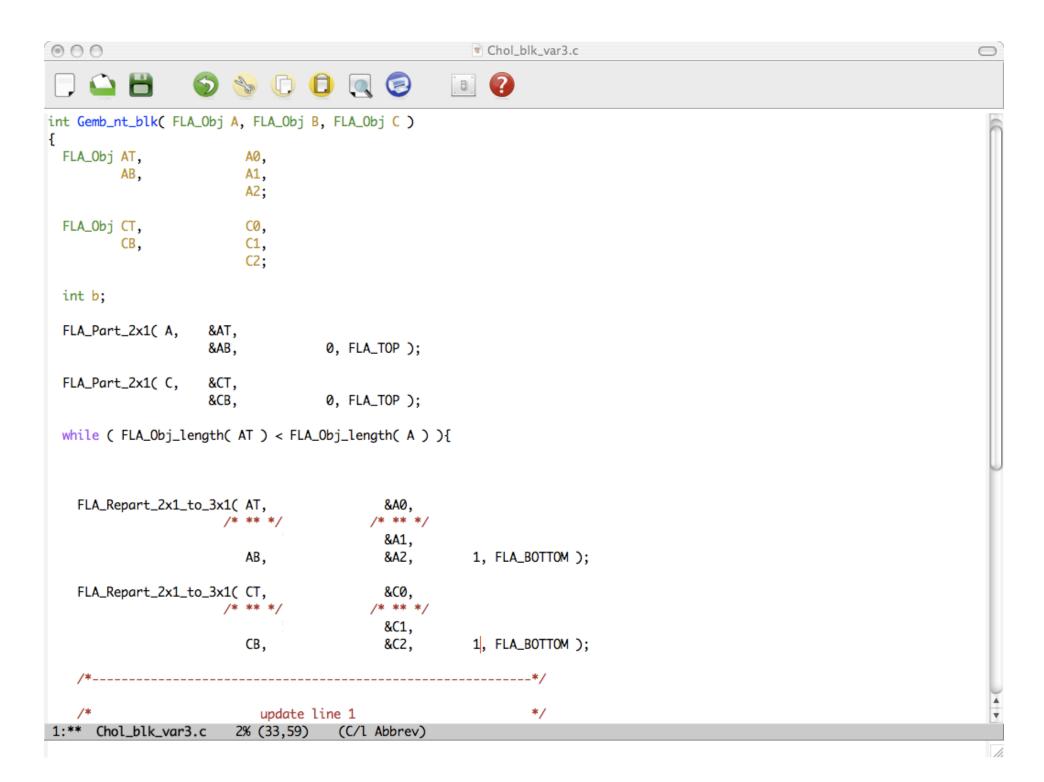


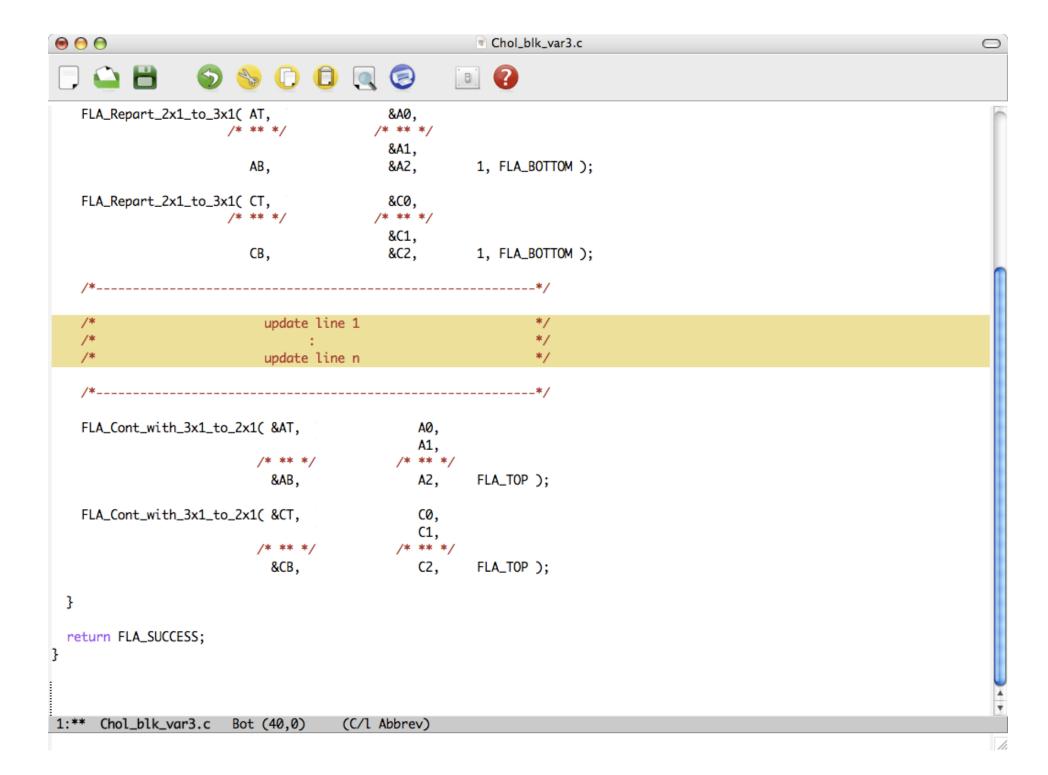


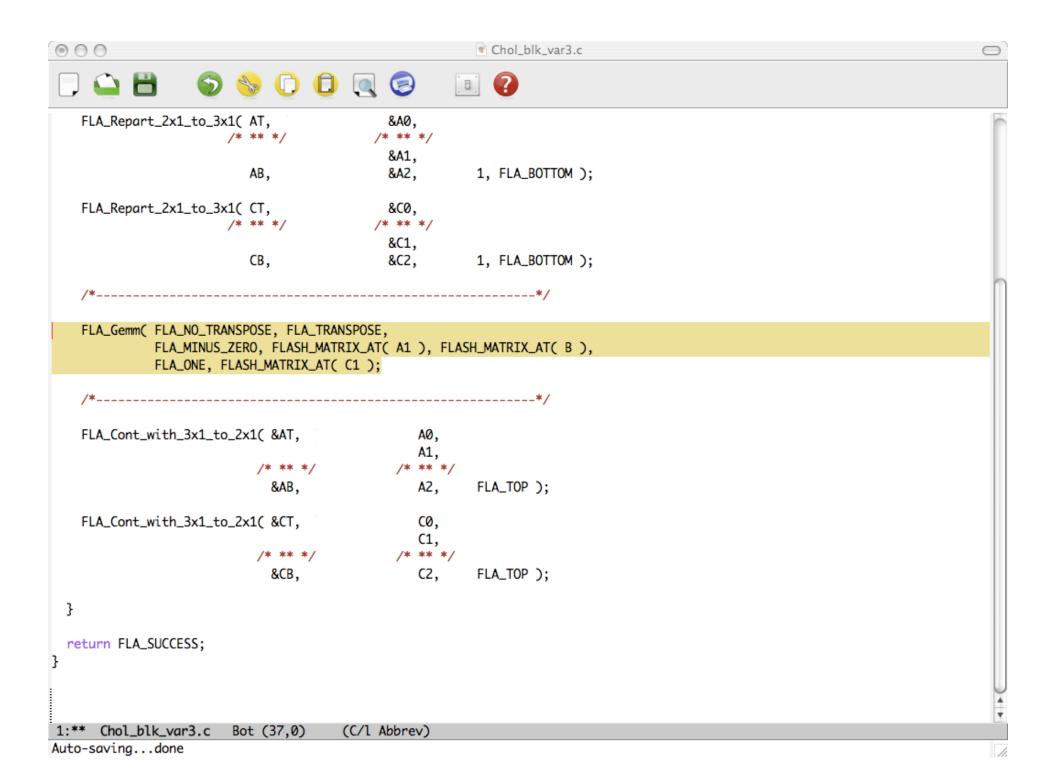




```
000
                                                      Chol_blk_var3.c
                                                                                                                        🕤 🦠 🕕 📵 📵 🤕
int Gemb_nt_blk( FLA_Obj A, FLA_Obj B, FLA_Obj C, int nb_alg )
 FLA_Obj AT,
                         Α0,
                         A1,
         AB,
                         A2;
 FLA_Obj CT,
                         C0,
         CB,
                         C1,
                         C2;
 int b;
 FLA_Part_2x1( A,
                    &ΑT,
                                0, FLA_TOP );
                    &AB,
 FLA_Part_2x1( C,
                    &CT,
                              0, FLA_TOP );
                    &CB,
 while ( FLA_Obj_length( AT ) < FLA_Obj_length( A ) ){</pre>
   b = min( FLA_Obj_length( AB ), nb_alg );
                                           &A0,
   FLA_Repart_2x1_to_3x1( AT,
                                         /* ** */
                      /* ** */
                                           &A1,
                         AB,
                                           &A2,
                                                      b, FLA_BOTTOM );
   FLA_Repart_2x1_to_3x1( CT,
                                          &C0,
                                        /* ** */
                      /* ** */
                                           &C1,
                         CB,
                                           &C2,
                                                      b, FLA_BOTTOM );
                                                              */
                           update line 1
1:** Chol_blk_var3.c
                     2% (3,60)
                                     (C/l Abbrev)
```







# Done!

#### Overview

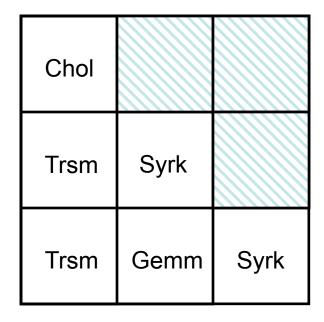
- A bit of history
- Programming algorithms-by-blocks is hard easy
  - An example: Cholesky factorization by blocks
- Programming algorithms-by-blocks further simplifies complicates programming (future) multicore architectures
- Conclusion
- Resources

## Programming Dense-Matrix on Multicore is hard easy

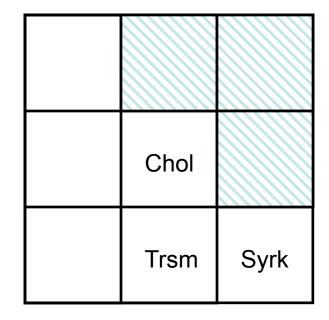
### The basic idea

- Algorithms-by-blocks
  - Unit of data is a block
  - Unit of computation is a (BLAS-like) operation with blocks
  - Apply superscalar techniques at the block level
  - In software (runtime system) rather than hardware

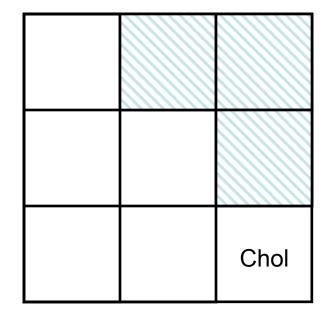
- Cholesky Factorization
  - Iteration 1



- Cholesky Factorization
  - Iteration 2



- Cholesky Factorization
  - Iteration 3

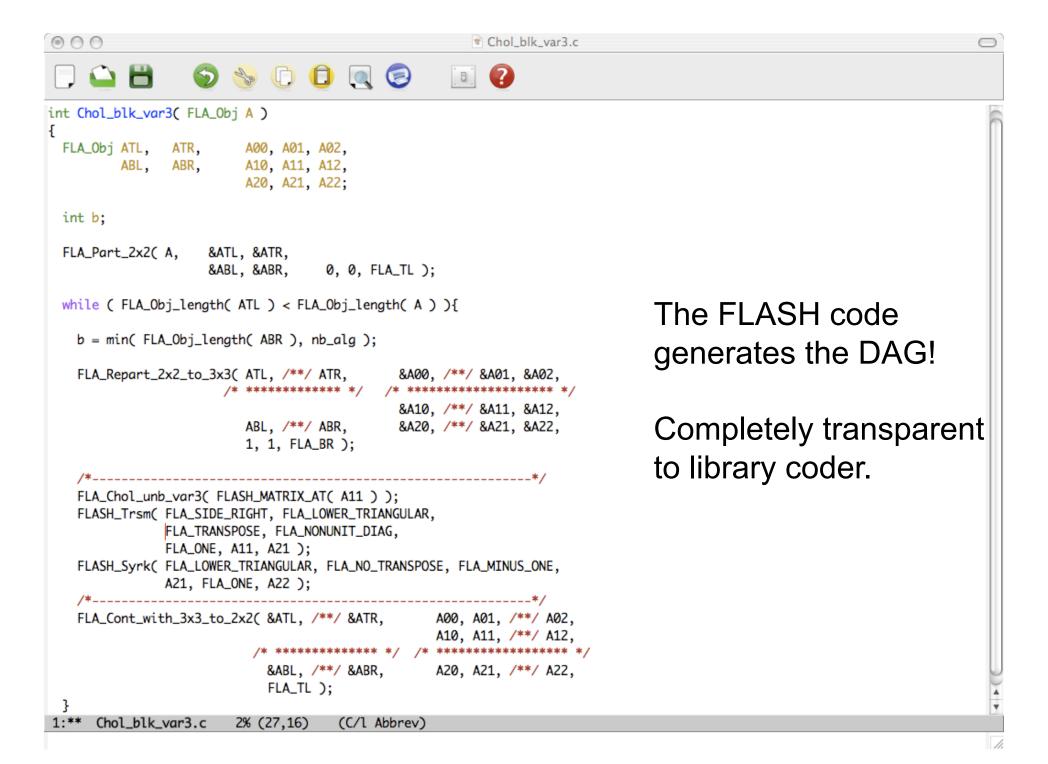


## Basic idea (continued)

- Analyzer:
  - Build the DAG: Calls like

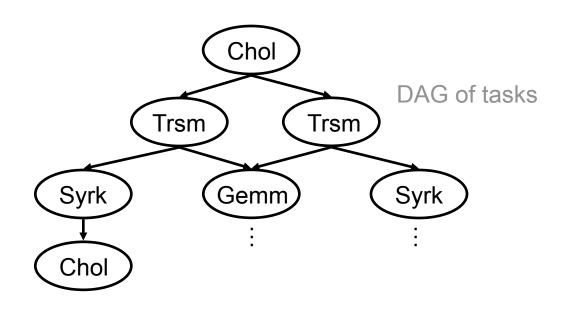
```
FLA_Chol (FLA_LOWER_TRIANGULAR, FLASH_MATRIX_AT (A11))
place a tasks on a queue
```

- DAG: nodes are tasks, edges are dependencies.
- At run time check if dependencies have been met. Schedule tasks to threads.
- Akin to Tomasulo's algorithm and instructionlevel parallelism on blocks of computation
- Runtime system: SuperMatrix



#### Analyzer

Task Queue
Trsm
Trsm
Syrk
Gemm
Syrk
Chol
:
June 19, 2008



ORNL 08

www.cs.utexas.edu/users/flame/

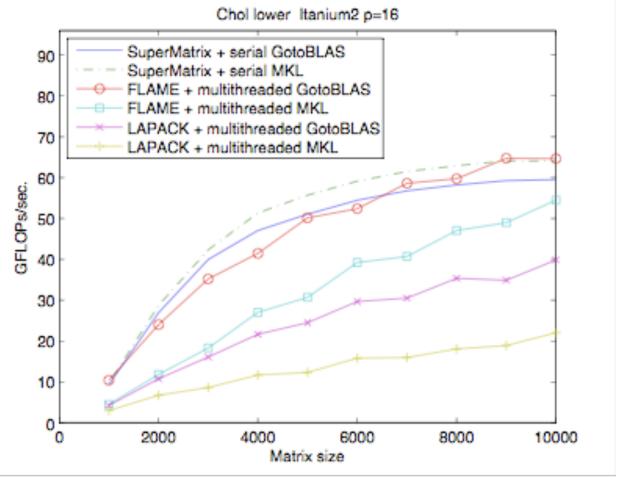
- Dispatcher
  - Use DAG to execute tasks out-of-order in parallel
  - Akin to Tomasulo's algorithm and instruction-level parallelism on blocks of computation
    - SuperScalar vs. SuperMatrix

- Dispatcher
  - -4 threads
  - 5 x 5 matrixof blocks
  - 35 tasks
  - 14 stages

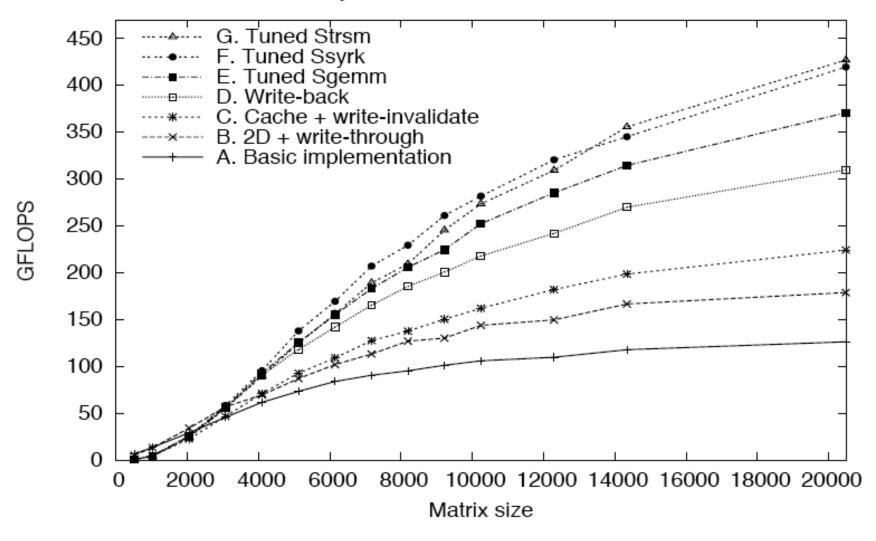
Chol			
Trsm	Trsm	Trsm	Trsm
Syrk	Gemm	Syrk	Gemm
Gemm	Syrk	Gemm	Gemm
Gemm	Syrk	Chol	
Trsm	Trsm	Trsm	
Syrk	Gemm	Syrk	Gemm
Gemm	Syrk	Chol	
Trsm	Trsm		
Syrk	Gemm	Syrk	
Chol			
Trsm			
Syrk			
Chol	V	vww.cs.utexas	edu/users/flan

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### Performance



#### Cholesky factorization on NVIDIA Tesla S870



## Scope of Methodology

- Implemented so far:
  - Cholesky: A few weeks (includes writing the SuperMatrix runtime system)
  - BLAS3: 2 people, 1 weekend
  - LU-by-blocks with incremental pivoting: 1 person, a few days
  - QR factorization-by-blocks: 1 person, a few days
  - Solution of triangular Sylvester equation: 1 person, a few days

#### Overview

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### Conclusion

- Is it time to stop evolving from LINPACK?
- Coding at a high level of abstraction yields a more flexible design
- The time for algorithms-by-blocks appears to have arrived
- Often new algorithms are required to support algorithms by blocks

### Resources



The Science of Programming Matrix Computations

by

Robert A. van de Geijn

The University of Texas at Austin and

Enrique S. Quintana-Ortí

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